

VISIT...

LANZAROTE  
*Caliente*.COM

---

# LANGE'S HANDBOOK OF CHEMISTRY

---

**John A. Dean**

*Professor Emeritus of Chemistry  
University of Tennessee, Knoxville*

**Fifteenth Edition**

**McGRAW-HILL, INC.**

New York St. Louis San Francisco Auckland Bogotá  
Caracas Lisbon London Madrid Mexico Milan  
Montreal New Delhi Paris San Juan São Paulo  
Singapore Sydney Tokyo Toronto

Copyright © 1999, 1992, 1985, 1979, 1973, 1967, 1961, 1956 by McGraw-Hill, Inc. All rights reserved.

Copyright renewed 1972 by Norbert Adolph Lange.

Copyright 1952, 1949, 1946, 1944, 1941, 1939, 1937, 1934 by McGraw-Hill, Inc. All rights reserved. Printed in the United States of America. Except as permitted under the United States Copyright Act of 1976, no part of this publication may be reproduced or distributed in any form or by any means, or stored in a data base retrieval system without the prior written permission of the publisher.

5 6 7 8 9 0 DOC/DOC 9 0 3 2 1 0 9 8

ISBN 0-07-016384-7

*The sponsoring editor for this book was Robert Esposito, and the production supervisor was Clare B. Stanley. It was set in Times Roman by Progressive Information Technologies.*

*Printed and bound by R. R. Donnelley & Sons Company.*

Information contained in this work has been obtained by McGraw-Hill, Inc., from sources believed to be reliable. However, neither McGraw-Hill nor its authors guarantee the accuracy or completeness of any information published herein and neither McGraw-Hill nor its authors shall be responsible for any errors, omissions, or damages arising out of use of this information. This work is published with the understanding that McGraw-Hill and its authors are supplying information but are not attempting to render engineering or other professional services. If such services are required, the assistance of an appropriate profession should be sought.

---

# ACKNOWLEDGMENTS

---

Grateful acknowledgment is hereby made of an indebtedness to those who have contributed to previous editions and whose compilations continue in use in this edition. In particular, acknowledgment is made of the contribution of L. P. Buseth, who prepared the conversion tables for the thirteenth edition and who prepared the table on the U.S. Standard Sieve Series.

---

## ABOUT THE EDITOR

---

John A. Dean assumed the editorship of *Lange's Handbook of Chemistry* in 1968 with the Eleventh Edition. He is currently Professor Emeritus of Chemistry at the University of Tennessee at Knoxville. The author of nine major chemistry reference books used throughout the world, John Dean's research interests, reflected in over 105 research papers and scholarly publications, include instrumental methods of analysis, flame emission and atomic absorption spectroscopy, chromatographic and solvent extraction methods, and polarography. He received his B.S., M.S., and Ph.D. in Chemistry from the University of Michigan at Ann Arbor. In 1974, he was given the Charles H. Stone Award by the Carolina-Piedmont Section of the American Chemical Society. In 1991, he was awarded the Distinguished Service Award by the Society for Applied Spectroscopy; by the same organization he was awarded Honorary Membership in 1997.

---

# PREFACE TO FIFTEENTH EDITION

---

This new edition, the fifth under the aegis of the present editor, remains the one-volume source of factual information for chemists, both professionals and students—the first place in which to “look it up” on the spot. The aim is to provide sufficient data to satisfy all one’s general needs without recourse to other reference sources. A user will find this volume of value as a time-saver because of the many tables of numerical data which have been especially compiled.

Descriptive properties for a basic group of approximately 4300 organic compounds are compiled in Section 1, an increase of 300 entries. All entries are listed alphabetically according to the senior prefix of the name. The data for each organic compound include (where available) name, structural formula, formula weight, Beilstein reference (or if unavailable, the entry to the *Merck Index*, 12th ed.), density, refractive index, melting point, boiling point, flash point, and solubility (citing numerical values if known) in water and various common organic solvents. Structural formulas either too complex or too ambiguous to be rendered as line formulas are grouped at the bottom of each facing double page on which the entries appear. Alternative names, as well as trivial names of long-standing usage, are listed in their respective alphabetical order at the bottom of each double page in the regular alphabetical sequence. Another feature that assists the user in locating a desired entry is the empirical formula index.

Section 2 on General Information, Conversion Tables, and Mathematics has had the table on general conversion factors thoroughly reworked. Similarly the material on Statistics in Chemical Analysis has had its contents more than doubled.

Descriptive properties for a basic group of inorganic compounds are compiled in Section 3, which has undergone a small increase in the number of entries. Many entries under the column “Solubility” supply the reader with precise quantities dissolved in a stated solvent and at a given temperature.

Several portions of Section 4, Properties of Atoms, Radicals, and Bonds, have been significantly enlarged. For example, the entries under “Ionization Energy of Molecular and Radical Species” now number 740 and have an additional column with the enthalpy of formation of the ions. Likewise, the table on “Electron Affinities of the Elements, Molecules, and Radicals” now contains about 225 entries. The Table of Nuclides has material on additional radionuclides, their radiations, and the neutron capture cross sections.

Revised material for Section 5 includes the material on surface tension, viscosity, dielectric constant, and dipole moment for organic compounds. In order to include more data at several temperatures, the material has been divided into two separate tables. Material on surface tension and viscosity constitute the first table with 715 entries; included is the temperature range of the liquid phase. Material on dielectric constant and dipole

moment constitute another table of 1220 entries. The additional data at two or more temperatures permit interpolation for intermediate temperatures and also permit limited extrapolation of the data. The Properties of Combustible Mixtures in Air has been revised and expanded to include over 450 compounds. Flash points are to be found in Section 1. Completely revised are the tables on Thermal Conductivity for gases, liquids, and solids. Van der Waals' constants for gases has been brought up to date and expanded to over 500 substances.

Section 6, which includes Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic and Inorganic Compounds, and Heats of Melting, Vaporization, and Sublimation and Specific Heat at Various Temperatures for organic and inorganic compounds, has expanded by 11 pages, but the major additions have involved data in columns where it previously was absent. More material has also been included for critical temperature, critical pressure, and critical volume.

The section on Spectroscopy has been retained but with some revisions and expansion. The section includes ultraviolet-visible spectroscopy, fluorescence, infrared and Raman spectroscopy, and X-ray spectrometry. Detection limits are listed for the elements when using flame emission, flame atomic absorption, electrothermal atomic absorption, argon induction coupled plasma, and flame atomic fluorescence. Nuclear magnetic resonance embraces tables for the nuclear properties of the elements, proton chemical shifts and coupling constants, and similar material for carbon-13, boron-11, nitrogen-15, fluorine-19, silicon-29, and phosphorus-31.

In Section 8, the material on solubility constants has been doubled to 550 entries. Sections on proton transfer reactions, including some at various temperatures, formation constants of metal complexes with organic and inorganic ligands, buffer solutions of all types, reference electrodes, indicators, and electrode potentials are retained with some revisions. The material on conductances has been revised and expanded, particularly in the table on limiting equivalent ionic conductances.

Everything in Sections 9 and 10 on physiochemical relationships, and on polymers, rubbers, fats, oils, and waxes, respectively, has been retained.

Section 11, Practical Laboratory Information, has undergone significant changes and expansion. Entries in the table on "Molecular Elevation of the Boiling Point" have been increased. McReynolds' constants for stationary phases in gas chromatography have been reorganized and expanded. The guide to ion-exchange resins and discussion is new and embraces all types of column packings and membrane materials. Gravimetric factors have been altered to reflect the changes in atomic weights for several elements. Newly added are tables listing elements precipitated by general analytical reagents, and giving equations for the redox determination of the elements with their equivalent weights. Discussion on the topics of precipitation and complexometric titrations include primary standards and indicators for each analytical technique. A new topic of masking and demasking agents includes discussion and tables of masking agents for various elements, for anions and neutral molecules, and common demasking agents. A table has been added listing the common amino acids with their pI and  $pK_a$  values and their 3-letter and 1-letter abbreviations. Lastly a 9-page table lists the threshold limit value (TLV) for gases and vapors.

As stated in earlier prefaces, every effort has been made to select the most useful and reliable information and to record it with accuracy. However, the editor's 50 years of

involvement with textbooks and handbooks bring a realization of the opportunities for gremlins to exert their inevitable mischief. It is hoped that users of this handbook will continue to offer suggestions of material that might be included in, or even excluded from, future editions and call attention to errors. These communications should be directed to the editor. The street address will change early in 1999, as will the telephone number. However, the e-mail address should remain as “pd105@aol.com.”

*Knoxville, TN*

*John A. Dean*



---

# PREFACE TO FOURTEENTH EDITION

---

Perhaps it would be simplest to begin by stating the ways in which this new edition, the fourth under the aegis of the present editor, has *not* been changed. It remains the one-volume source of factual information for chemists, both professionals and students—the first place in which to “look it up” on the spot. The aim is to provide sufficient data to satisfy all one’s general needs without recourse to other reference sources. Even the worker with the facilities of a comprehensive library will find this volume of value as a time-saver because of the many tables of numerical data which have been especially compiled.

The changes, however, are both numerous and significant. First of all, there is a change in the organization of the subject matter. For example, material formerly contained in the section entitled Analytical Chemistry is now grouped by operational categories: spectroscopy; electrolytes, electromotive force, and chemical equilibrium; and practical laboratory information. Polymers, rubbers, fats, oils, and waxes constitute a large independent section.

Descriptive properties for a basic group of approximately 4000 organic compounds are compiled in Section 1. These follow a concise introduction to organic nomenclature, including the topic of stereochemistry. Nomenclature is consistent with the 1979 rules of the Commission on Nomenclature, International Union of Pure and Applied Chemistry (IUPAC). All entries are listed alphabetically according to the senior prefix of the name. The data for each organic compound include (where available) name, structural formula, formula weight, Beilstein reference, density, refractive index, melting point, boiling point, flash point, and solubility (citing numerical values if known) in water and various common organic solvents. Structural formulas either too complex or too ambiguous to be rendered as line formulas are grouped at the bottom of the page on which the entries appear. Alternative names, as well as trivial names of long-standing usage, are listed in their respective alphabetical order at the bottom of each page in the regular alphabetical sequence. Another feature that assists the user in locating a desired entry is the empirical formula index.

Section 2 combines the former separate section on Mathematics with the material involving General Information and Conversion Tables. The fundamental physical constants reflect values recommended in 1986. Physical and chemical symbols and definitions have undergone extensive revision and expansion. Presented in 14 categories, the entries follow recommendations published in 1988 by the IUPAC. The table of abbreviations and standard letter symbols provides, in a sense, an alphabetical index to the foregoing tables. The table of conversion factors has been modified in view of recent data and inclusion of SI units; cross-entries for “archaic” or unusual entries have been curtailed.

Descriptive properties for a basic group of approximately 1400 inorganic compounds are compiled in Section 3. These follow a concise, revised introduction to inorganic nomenclature that follows the recommendations of the IUPAC published in 1990. In this section are given the exact atomic (or formula) weight of the elements accompanied, when available, by the uncertainty in the final figure given in parentheses.

In Section 4 the data on bond lengths and strengths have been vastly increased so as to include not only the atomic and effective ionic radii of elements and the covalent radii for atoms, but also the bond lengths between carbon and other elements and between elements other than carbon. All

lengths are given in picometers (SI unit). Effective ionic radii are tabulated as a function of ion charge and coordination number. Bond dissociation energies are given in kilojoules per mole with the uncertainty of the final figure(s) given in parentheses when known. New tables include bond dipole moments, group dipole moments, work functions of the elements, and relative abundances of the naturally occurring elements. The table of nuclides has been shortened and includes only the more commonly encountered nuclides; tabulations list half-life, natural abundance, cross-section to thermal neutrons, and radiation emitted upon disintegration. Entries have been updated.

Revised material in Section 5 includes an extensive tabulation of binary and ternary azeotropes comprising approximately 850 entries. Over 975 compounds have values listed for viscosity, dielectric constant, dipole moment, and surface tension. Whenever possible, data for viscosity and dielectric constant are provided at two temperatures to permit interpolation for intermediate temperatures and also to permit limited extrapolation of the data. The dipole moments are often listed for different physical states. Values for surface tension can be calculated over a range of temperatures from two constants that can be fitted into a linear equation. Also extensively revised and expanded are the properties of combustible mixtures in air. A table of triple points has been added.

The tables in Section 6 contain values of the enthalpy and Gibbs energy of formation, entropy, and heat capacity at five temperatures for approximately 2000 organic compounds and 1500 inorganic compounds, many in more than one physical state. Separate tabulations have enthalpies of melting, vaporization, transition, and sublimation for organic and inorganic compounds. All values are given in SI units (joule) and have been extracted from the latest sources such as *JANAF Thermochemical Tables*, 3d ed. (1986); *Thermochemical Data of Organic Compounds*, 2d ed. (1986); and *Enthalpies of Vaporization of Organic Compounds*, published under the auspices of the IUPAC (1985). Also updated is the material on critical properties of elements and compounds.

The section on Spectroscopy has been expanded to include ultraviolet-visible spectroscopy, fluorescence, Raman spectroscopy, and mass spectroscopy. Retained sections have been thoroughly revised: in particular, the tables on electronic emission and atomic absorption spectroscopy, nuclear magnetic resonance, and infrared spectroscopy. Detection limits are listed for the elements when using flame emission, flame atomic absorption, electrothermal atomic absorption, argon ICP, and flame atomic fluorescence. Nuclear magnetic resonance embraces tables for the nuclear properties of the elements, proton chemical shifts and coupling constants, and similar material for carbon-13, boron-11, nitrogen-15, fluorine-19, silicon-29, and phosphorus-31.

Section 8 now combines all the material on electrolytes, electromotive force, and chemical equilibrium, some of which had formerly been included in the old "Analytical Chemistry" section of earlier editions. Material on the half-wave potentials of inorganic and organic materials has been thoroughly revised. The tabulation of the potentials of the elements and their compounds reflects recent IUPAC (1985) recommendations.

An extensive new Section 10 is devoted to polymers, rubbers, fats, oils, and waxes. A discussion of polymers and rubbers is followed by the formulas and key properties of plastic materials. For each member and type of the plastic families there is a tabulation of their physical, electrical, mechanical, and thermal properties and characteristics. A similar treatment is accorded the various types of rubber materials. Chemical resistance and gas permeability constants are also given for rubbers and plastics. The section concludes with various constants of fats, oils, and waxes.

The practical laboratory information contained in Section 11 has been gathered from many of the previous sections of earlier editions. This material has been supplemented with new material under separation methods, gravimetric and volumetric analysis, and laboratory solutions. Significant new tables under separation methods include: properties of solvents for chromatography, solvents having the same refractive index and the same density, McReynolds' constants for stationary phases in gas chromatography, characteristics of selected supercritical fluids, and typical performances in HPLC for various operating conditions. Under gravimetric and volumetric analysis, gravimetric factors, equations and equivalents for volumetric analysis, and titrimetric factors have been retained

along with the formation constants of EDTA metal complexes. In this age of awareness of chemical dangers, tables have been added for some common reactive and incompatible chemicals, chemicals recommended for refrigerated storage, and chemicals which polymerize or decompose on extended storage at low temperature. Updated is the information about the U.S. Standard Sieve Series. Thermometry data have been revised to bring them into agreement with the new International Temperature Scale–1990, and data for type N thermocouples are included.

Every effort has been made to select the most useful and most reliable information and to record it with accuracy. However, the editor's many years of involvement with handbooks bring a realization of the opportunities for gremlins to exert their inevitable mischief. It is hoped that users of this handbook will offer suggestions of material that might be included in, or even excluded from, future editions and call attention to errors. These communications should be directed to the editor at his home address (or by telephone).

*John A. Dean*

---

# PREFACE TO FIRST EDITION

---

This book is the result of a number of years' experience in the compiling and editing of data useful to chemists. In it an effort has been made to select material to meet the needs of chemists who cannot command the unlimited time available to the research specialist, or who lack the facilities of a large technical library which so often is not conveniently located at many manufacturing centers. If the information contained herein serves this purpose, the compiler will feel that he has accomplished a worthy task. Even the worker with the facilities of a comprehensive library may find this volume of value as a time-saver because of the many tables of numerical data which have been especially computed for this purpose.

Every effort has been made to select the most reliable information and to record it with accuracy. Many years of occupation with this type of work bring a realization of the opportunities for the occurrence of errors, and while every endeavor has been made to prevent them, yet it would be remarkable if the attempts towards this end had always been successful. In this connection it is desired to express appreciation to those who in the past have called attention to errors, and it will be appreciated if this be done again with the present compilation for the publishers have given their assurance that no expense will be spared in making the necessary changes in subsequent printings.

It has been aimed to produce a compilation complete within the limits set by the economy of available space. One difficulty always at hand to the compiler of such a book is that he must decide what data are to be excluded in order to keep the volume from becoming unwieldy because of its size. He can hardly be expected to have an expert's knowledge of all branches of the science nor the intuition necessary to decide in all cases which particular value to record, especially when many differing values are given in the literature for the same constant. If the expert in a particular field will judge the usefulness of this book by the data which it supplies to him from fields other than his specialty and not by the lack of highly specialized information in which only he and his co-workers are interested (and with which he is familiar and for which he would never have occasion to consult this compilation), then an estimate of its value to him will be apparent. However, if such specialists will call attention to missing data with which they are familiar and which they believe others less specialized will also need, then works of this type can be improved in succeeding editions.

Many of the gaps in this volume are caused by the lack of such information in the literature. It is hoped that to one of the most important classes of workers in chemistry, namely the teachers, the book will be of value not only as an aid in answering the most varied questions with which they are confronted by interested students, but also as an inspiration through what it suggests by the gaps and inconsistencies, challenging as they do the incentive to engage in the creative and experimental work necessary to supply the missing information.

While the principal value of the book is for the professional chemist or student of chemistry, it should also be of value to many people not especially educated as chemists. Workers in the natural sciences—physicists, mineralogists, biologists, pharmacists, engineers, patent attorneys, and librarians—are often called upon to solve problems dealing with the properties of chemical products or materials of construction. For such needs this compilation supplies helpful information and will serve not only as an economical substitute for the costly accumulation of a large library of monographs on specialized subjects, but also as a means of conserving the time required to search for

information so widely scattered throughout the literature. For this reason especial care has been taken in compiling a comprehensive index and in furnishing cross references with many of the tables.

It is hoped that this book will be of the same usefulness to the worker in science as is the dictionary to the worker in literature, and that its resting place will be on the desk rather than on the bookshelf.

*Cleveland, Ohio*  
*May 2, 1934*

*N. A. Lange*

---

# CONTENTS

---

*For the detailed contents of any section, consult the title page of that section. See also the alphabetical index in the back of this handbook.*

Preface to Fifteenth Edition      vii

Preface to Fourteenth Edition

Preface to First Edition      xv

Acknowledgments      xvii

|             |                                                             |      |
|-------------|-------------------------------------------------------------|------|
| Section 1.  | Organic Compounds                                           | 1.1  |
| Section 2.  | General Information, Conversion Tables, and Mathematics     | 2.1  |
| Section 3.  | Inorganic Compounds                                         | 3.1  |
| Section 4.  | Properties of Atoms, Radicals, and Bonds                    | 4.1  |
| Section 5.  | Physical Properties                                         | 5.1  |
| Section 6.  | Thermodynamic Properties                                    | 6.1  |
| Section 7.  | Spectroscopy                                                | 7.1  |
| Section 8.  | Electrolytes, Electromotive Force, and Chemical Equilibrium | 8.1  |
| Section 9.  | Physicochemical Relationships                               | 9.1  |
| Section 10. | Polymers, Rubbers, Fats, Oils, and Waxes                    | 10.1 |
| Section 11. | Practical Laboratory Information                            | 11.1 |

Index follows Section 11

---

# SECTION 1

---

## ORGANIC COMPOUNDS

---

|                                                                                                   |             |
|---------------------------------------------------------------------------------------------------|-------------|
| <b>1.1 NOMENCLATURE OF ORGANIC COMPOUNDS</b>                                                      | <b>1.1</b>  |
| <b>1.1.1 Nonfunctional Compounds</b>                                                              | <b>1.1</b>  |
| Table 1.1 Names of Straight-Chain Alkanes                                                         | 1.2         |
| Table 1.2 Fused Polycyclic Hydrocarbons                                                           | 1.8         |
| Table 1.3 Specialist Nomenclature for Heterocyclic Systems                                        | 1.11        |
| Table 1.4 Suffixes for Specialist Nomenclature of Heterocyclic Systems                            | 1.12        |
| Table 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names                  | 1.13        |
| Table 1.6 Trivial Names for Heterocyclic Systems That Are Not Recommended for Use in Fusion Names | 1.16        |
| <b>1.1.2 Functional Compounds</b>                                                                 | <b>1.17</b> |
| Table 1.7 Characteristic Groups for Substitutive Nomenclature                                     | 1.18        |
| Table 1.8 Characteristic Groups Cited Only as Prefixes in Substitutive Nomenclature               | 1.19        |
| Table 1.9 Functional Class Names Used in Radicofunctional Nomenclature                            | 1.22        |
| <b>1.1.3 Specific Functional Groups</b>                                                           | <b>1.23</b> |
| Table 1.10 Retained Trivial Names of Alcohols and Phenols with Structures                         | 1.24        |
| Table 1.11 Names of Some Carboxylic Acids                                                         | 1.30        |
| Table 1.12 Parent Structures of Phosphorus-Containing Compounds                                   | 1.36        |
| <b>1.1.4 Stereochemistry</b>                                                                      | <b>1.39</b> |
| <b>1.1.5 Chemical Abstracts Indexing System</b>                                                   | <b>1.49</b> |
| Table 1.13 Names and Formulas of Organic Radicals                                                 | 1.51        |
| <b>1.2 PHYSICAL PROPERTIES OF PURE SUBSTANCES</b>                                                 | <b>1.58</b> |
| Table 1.14 Empirical Formula Index of Organic Compounds                                           | 1.58        |
| Table 1.15 Physical Constants of Organic Compounds                                                | 1.74        |

---

### 1.1 NOMENCLATURE OF ORGANIC COMPOUNDS

---

The following synopsis of rules for naming organic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see J. Rigaudy and S. P. Klesney, *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979. This publication contains the recommendations of the Commission on Nomenclature of Organic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).

#### 1.1.1 Nonfunctional Compounds

**1.1.1.1 Alkanes.** The saturated open-chain (acyclic) hydrocarbons ( $C_nH_{2n+2}$ ) have names ending in -ane. The first four members have the trivial names *methane* ( $CH_4$ ), *ethane* ( $CH_3CH_3$  or  $C_2H_6$ ), *propane* ( $C_3H_8$ ), and *butane* ( $C_4H_{10}$ ). For the remainder of the alkanes, the first portion of the name

is derived from the Greek prefix (see Table 2.4) that cites the number of carbons in the alkane followed by -ane with elision of the terminal -a from the prefix, as shown in Table 1.1.

**TABLE 1.1** Names of Straight-Chain Alkanes

| $n^*$ | Name    | $n^*$ | Name        | $n^*$ | Name           | $n^*$ | Name            |
|-------|---------|-------|-------------|-------|----------------|-------|-----------------|
| 1     | Methane | 11    | Undecane‡   | 21    | Henicosane     | 60    | Hexacontane     |
| 2     | Ethane  | 12    | Dodecane    | 22    | Docosane       | 70    | Heptacontane    |
| 3     | Propane | 13    | Tridecane   | 23    | Tricosane      | 80    | Octacontane     |
| 4     | Butane  | 14    | Tetradecane |       |                | 90    | Nonacontane     |
| 5     | Pentane | 15    | Pentadecane | 30    | Triacontane    | 100   | Hectane         |
| 6     | Hexane  | 16    | Hexadecane  | 31    | Hentriacontane | 110   | Decahectane     |
| 7     | Heptane | 17    | Heptadecane | 32    | Dotriacontane  | 120   | Icosahectane    |
| 8     | Octane  | 18    | Octadecane  |       |                | 121   | Henicosahectane |
| 9     | Nonane† | 19    | Nonadecane  | 40    | Tetracontane   |       |                 |
| 10    | Decane  | 20    | Icosane§    | 50    | Pentacontane   |       |                 |

\*  $n$  = total number of carbon atoms.

† Formerly called enneane.

‡ Formerly called hendecane.

§ Formerly called eicosane.

For branching compounds, the parent structure is the longest continuous chain present in the compound. Consider the compound to have been derived from this structure by replacement of hydrogen by various alkyl groups. Arabic number prefixes indicate the carbon to which the alkyl group is attached. Start numbering at whichever end of the parent structure that results in the lowest-numbered locants. The arabic prefixes are listed in numerical sequence, separated from each other by commas and from the remainder of the name by a hyphen.

If the same alkyl group occurs more than once as a side chain, this is indicated by the prefixes di-, tri-, tetra-, etc. Side chains are cited in alphabetical order (before insertion of any multiplying prefix). The name of a complex radical (side chain) is considered to begin with the first letter of its complete name. Where names of complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest-numbered locant at the first cited point of difference in the radical. If two or more side chains are in equivalent positions, the one to be assigned the lowest-numbered locant is that cited first in the name. The complete expression for the side chain may be enclosed in parentheses for clarity or the carbon atoms in side chains may be indicated by primed locants.

If hydrocarbon chains of equal length are competing for selection as the parent, the choice goes in descending order to (1) the chain that has the greatest number of side chains, (2) the chain whose side chains have the lowest-numbered locants, (3) the chain having the greatest number of carbon atoms in the smaller side chains, or (4) the chain having the least-branched side chains.

These trivial names may be used for the unsubstituted hydrocarbon only:

Isobutane  $(\text{CH}_3)_2\text{CHCH}_3$

Neopentane  $(\text{CH}_3)_4\text{C}$

Isopentane  $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$

Isohexane  $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3$

Univalent radicals derived from saturated unbranched alkanes by removal of hydrogen from a terminal carbon atom are named by adding -yl in place of -ane to the stem name. Thus the alkane

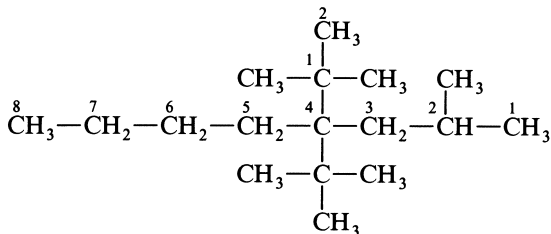
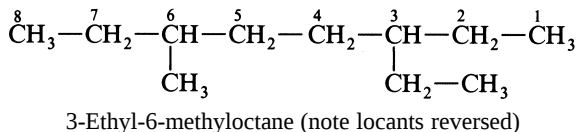
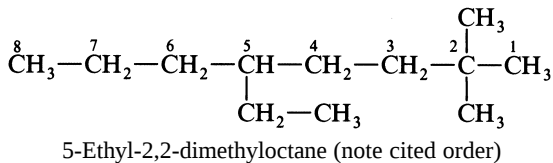
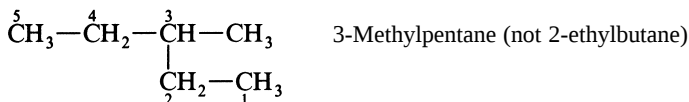
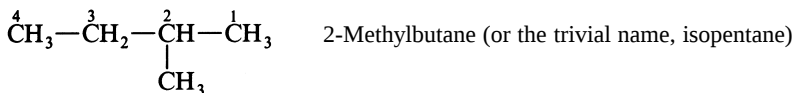


*ethane* becomes the radical *ethyl*. These exceptions are permitted for unsubstituted radicals only:

|                    |                                                 |                     |                                                       |
|--------------------|-------------------------------------------------|---------------------|-------------------------------------------------------|
| Isopropyl          | $(\text{CH}_3)_2\text{CH}-$                     | Isopentyl           | $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2-$            |
| Isobutyl           | $(\text{CH}_3)_2\text{CHCH}_2-$                 | Neopentyl           | $(\text{CH}_3)_3\text{CCH}_2-$                        |
| <i>sec</i> -Butyl  | $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-$ | <i>tert</i> -Pentyl | $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2-$      |
| <i>tert</i> -Butyl | $(\text{CH}_3)_3\text{C}-$                      | Isohexyl            | $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_2-$ |

Note the usage of the prefixes *iso*-, *neo*-, *sec*-, and *tert*-, and note when italics are employed. Italicized prefixes are never involved in alphabetization, except among themselves; thus *sec*-butyl would precede isobutyl, isohexyl would precede isopropyl, and *sec*-butyl would precede *tert*-butyl.

Examples of alkane nomenclature are



4,4-Bis(1,1-dimethylethyl)-2-methyloctane

4,4-Bis-1',1'-dimethylethyl-2-methyloctane

4,4-Bis(*tert*-butyl)-2-methyloctane

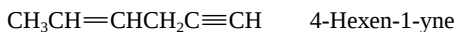
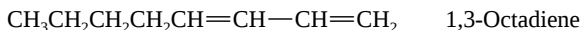
Bivalent radicals derived from saturated unbranched alkanes by removal of two hydrogen atoms are named as follows: (1) If both free bonds are on the same carbon atom, the ending -ane of the hydrocarbon is replaced with -ylidene. However, for the first member of the alkanes it is methylene

rather than methyldiene. Isopropylidene, *sec*-butylidene, and neopentylidene may be used for the unsubstituted group only. (2) If the two free bonds are on different carbon atoms, the straight-chain group terminating in these two carbon atoms is named by citing the number of methylene groups comprising the chain. Other carbon groups are named as substituents. Ethylene is used rather than dimethylene for the first member of the series, and propylene is retained for  $\text{CH}_3\text{—CH—CH}_2\text{—}$  (but trimethylene is  $\text{—CH}_2\text{—CH}_2\text{—CH}_2\text{—}$ ).

Trivalent groups derived by the removal of three hydrogen atoms from the same carbon are named by replacing the ending -ane of the parent hydrocarbon with -ylidyne.

**1.1.1.2 Alkenes and Alkynes.** Each name of the corresponding saturated hydrocarbon is converted to the corresponding alkene by changing the ending -ane to -ene. For alkynes the ending is -yne. With more than one double (or triple) bond, the endings are -adiene, -atriene, etc. (or -adiyne, -atriyne, etc.). The position of the double (or triple) bond in the parent chain is indicated by a locant obtained by numbering from the end of the chain nearest the double (or triple) bond; thus  $\text{CH}_3\text{CH}_2\text{CH=CH}_2$  is 1-butene and  $\text{CH}_3\text{C}\equiv\text{CCH}_3$  is 2-butyne.

For multiple unsaturated bonds, the chain is so numbered as to give the lowest possible locants to the unsaturated bonds. When there is a choice in numbering, the double bonds are given the lowest locants, and the alkene is cited before the alkyne where both occur in the name. Examples:

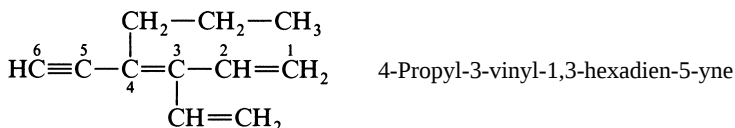


Unsaturated branched acyclic hydrocarbons are named as derivatives of the chain that contains the maximum number of double and/or triple bonds. When a choice exists, priority goes in sequence to (1) the chain with the greatest number of carbon atoms and (2) the chain containing the maximum number of double bonds.

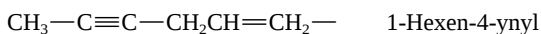
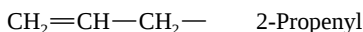
These nonsystematic names are retained:



An example of nomenclature for alkenes and alkynes is



Univalent radicals have the endings -enyl, -ynyl, -dienyl, -diynyl, etc. When necessary, the positions of the double and triple bonds are indicated by locants, with the carbon atom with the free valence numbered as 1. Examples:



These names are retained:

Vinyl (for ethenyl)  $\text{CH}_2=\text{CH}-$

Allyl (for 2-propenyl)  $\text{CH}_2=\text{CH}-\text{CH}_2-$

Isopropenyl (for 1-methylvinyl but for unsubstituted radical only)  $\text{CH}_2=\text{C}(\text{CH}_3)-$

Should there be a choice for the fundamental straight chain of a radical, that chain is selected which contains (1) the maximum number of double and triple bonds, (2) the largest number of carbon atoms, and (3) the largest number of double bonds. These are in descending priority.

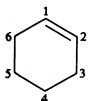
Bivalent radicals derived from unbranched alkenes, alkadienes, and alkynes by removing a hydrogen atom from each of the terminal carbon atoms are named by replacing the endings -ene, -diene, and -yne by -enylene, -dienylene, and -ynylene, respectively. Positions of double and triple bonds are indicated by numbers when necessary. The name *vinylene* instead of ethenylene is retained for  $-\text{CH}=\text{CH}-$ .

**1.1.1.3 Monocyclic Aliphatic Hydrocarbons.** Monocyclic aliphatic hydrocarbons (with no side chains) are named by prefixing cyclo- to the name of the corresponding open-chain hydrocarbon having the same number of carbon atoms as the ring. Radicals are formed as with the alkanes, alkenes, and alkynes. Examples:



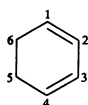
Cyclohexane

Cyclohexyl- (for the radical)



Cyclohexene

1-Cyclohexenyl- (for the radical with the free valence at carbon 1)

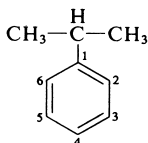


1,3-Cyclohexadiene

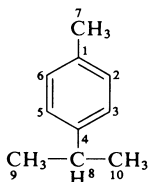
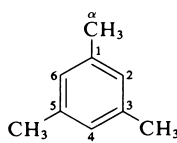
Cyclohexadienyl- (the unsaturated carbons are given numbers as low as possible, numbering from the carbon atom with the free valence given the number 1)

For convenience, aliphatic rings are often represented by simple geometric figures: a triangle for cyclopropane, a square for cyclobutane, a pentagon for cyclopentane, a hexagon (as illustrated) for cyclohexane, etc. It is understood that two hydrogen atoms are located at each corner of the figure unless some other group is indicated for one or both.

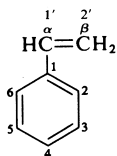
**1.1.1.4 Monocyclic Aromatic Compounds.** Except for six retained names, all monocyclic substituted aromatic hydrocarbons are named systematically as derivatives of benzene. Moreover, if the substituent introduced into a compound with a retained trivial name is identical with one already present in that compound, the compound is named as a derivative of benzene. These names are retained:



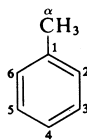
Cumene

Cymene (all three forms; *para*- shown)

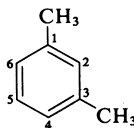
Mesitylene



Styrene



Toluene

Xylene (all three  
forms; *meta*- shown)

The position of substituents is indicated by numbers, with the lowest locant possible given to substituents. When a name is based on a recognized trivial name, priority for lowest-numbered locants is given to substituents implied by the trivial name. When only two substituents are present on a benzene ring, their position may be indicated by *o*- (*ortho*-), *m*- (*meta*-), and *p*- (*para*-) (and alphabetized in the order given) used in place of 1,2-, 1,3-, and 1,4-, respectively.

Radicals derived from monocyclic substituted aromatic hydrocarbons and having the free valence at a ring atom (numbered 1) are named phenyl (for benzene as parent, since benzyl is used for the radical  $\text{C}_6\text{H}_5\text{CH}_2-$ ), cumenyl, mesityl, tolyl, and xylyl. All other radicals are named as substituted phenyl radicals. For radicals having a single free valence in the side chain, these trivial names are retained:

Benzyl  $\text{C}_6\text{H}_5\text{CH}_2-$

Phenethyl  $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2-$

Benzhydryl (alternative to  
diphenylmethyl)  $(\text{C}_6\text{H}_5)_2\text{CH}-$

Styryl  $\text{C}_6\text{H}_5\text{CH}=\text{CH}-$

Cinnamyl  $\text{C}_6\text{H}_5\text{CH}=\text{CH}-\text{CH}_2-$

Trityl  $(\text{C}_6\text{H}_5)_3\text{C}-$

Otherwise, radicals having the free valence(s) in the side chain are named in accordance with the rules for alkanes, alkenes, or alkynes.

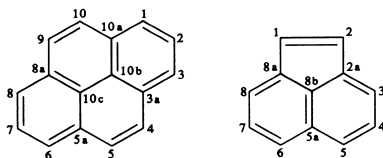
The name *phenylene* (*o*-, *m*-, or *p*-) is retained for the radical  $-\text{C}_6\text{H}_4-$ . Bivalent radicals formed from substituted benzene derivatives and having the free valences at ring atoms are named as substituted phenylene radicals, with the carbon atoms having the free valences being numbered 1,2-, 1,3-, or 1,4-, as appropriate.

Radicals having three or more free valences are named by adding the suffixes -triyl, -tetrayl, etc. to the systematic name of the corresponding hydrocarbon.

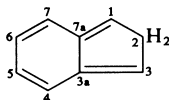
**1.1.1.5 Fused Polycyclic Hydrocarbons.** The names of polycyclic hydrocarbons containing the maximum number of conjugated double bonds end in -ene. Here the ending does not denote one double bond. Names of hydrocarbons containing five or more fused benzene rings in a linear arrangement are formed from a numerical prefix (see Table 2.4) followed by -acene. A partial list of the names of polycyclic hydrocarbons is given in Table 1.2. Many names are trivial.

Numbering of each ring system is fixed, as shown in Table 1.2, but it follows a systematic pattern. The individual rings of each system are oriented so that the greatest number of rings are (1) in a horizontal row and (2) the maximum number of rings are above and to the right (upper-right quadrant) of the horizontal row. When two orientations meet these requirements, the one is chosen that has the fewest rings in the lower-left quadrant. Numbering proceeds in a clockwise direction, commencing with the carbon atom not engaged in ring fusion that lies in the most counterclockwise position of the uppermost ring (upper-right quadrant); omit atoms common to two or more rings. Atoms common to two or more rings are designated by adding lowercase roman letters to the number of the position immediately preceding. Interior atoms follow the highest number, taking a clockwise

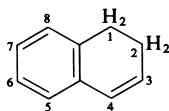
sequence wherever there is a choice. Anthracene and phenanthrene are two exceptions to the rule on numbering. Two examples of numbering follow:



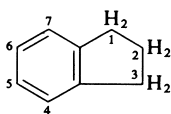
When a ring system with the maximum number of conjugated double bonds can exist in two or more forms differing only in the position of an “extra” hydrogen atom, the name can be made specific by indicating the position of the extra hydrogen(s). The compound name is modified with a locant followed by an italic capital *H* for each of these hydrogen atoms. Carbon atoms that carry an indicated hydrogen atom are numbered as low as possible. For example, 1*H*-indene is illustrated in Table 1.2; 2*H*-indene would be



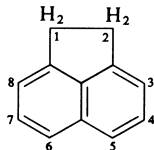
Names of polycyclic hydrocarbons with less than the maximum number of noncumulative double bonds are formed from a prefix dihydro-, tetrahydro-, etc., followed by the name of the corresponding unreduced hydrocarbon. The prefix perhydro- signifies full hydrogenation. For example, 1,2-dihydronaphthalene is



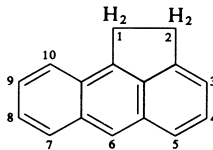
Examples of retained names and their structures are as follows:



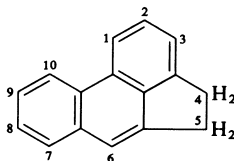
Indan



Acenaphthene



Aceanthrene

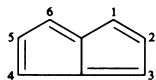


Acephenanthrene

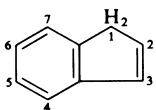
Polycyclic compounds in which two rings have two atoms in common or in which one ring contains two atoms in common with each of two or more rings of a contiguous series of rings and which contain at least two rings of five or more members with the maximum number of noncumu-

**TABLE 1.2** Fused Polycyclic Hydrocarbons*Listed in order of increasing priority for selection as parent compound.*

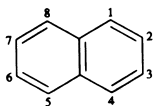
1. Pentalene



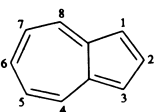
2. Indene



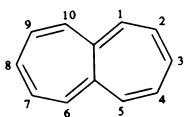
3. Naphthalene



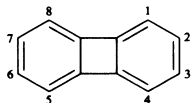
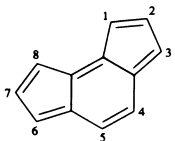
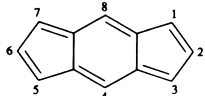
4. Azulene



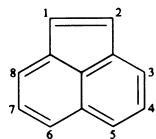
5. Heptalene



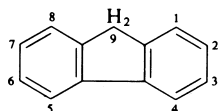
6. Biphenylene

7. *asym*-Indacene8. *sym*-Indacene

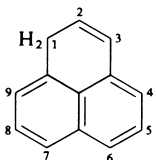
9. Acenaphthylene



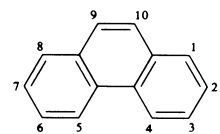
10. Fluorene



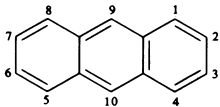
11. Phenalene



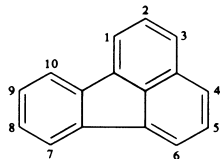
12. Phenanthrene\*



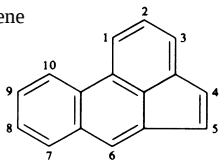
13. Anthracene\*



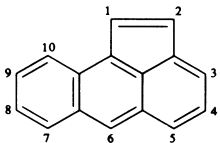
14. Fluoranthene



15. Acephenanthrylene

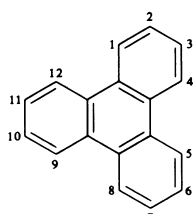
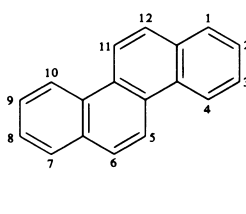
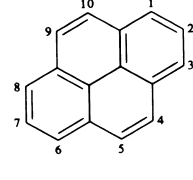
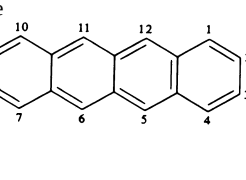


16. Aceanthrylene



\* Asterisk after a compound denotes exception to systematic numbering.

**TABLE 1.2** Fused Polycyclic Hydrocarbons (*Continued*)

|                                                                                                           |                                                                                                          |
|-----------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------|
| <p>17. Triphenylene</p>  | <p>19. Chrysene</p>     |
| <p>18. Pyrene</p>        | <p>20. Naphthacene</p>  |

lative double bonds and which have no accepted trivial name (Table 1.2) are named by prefixing to the name of the parent ring or ring system designations of the other components. The parent name should contain as many rings as possible (provided it has a trivial name) and should occur as far as possible from the beginning of the list in Table 1.2. Furthermore, the attached component(s) should be as simple as possible. For example, one writes dibenzophenanthrene and not naphthophenanthrene because the attached component benzo- is simpler than naphtho-. Prefixes designating attached components are formed by changing the ending -ene into -eno-; for example, indeno- from indene. Multiple prefixes are arranged in alphabetical order. Several abbreviated prefixes are recognized; the parent is given in parentheses:

Acenaphtho- (acenaphthylene)

Naphtho- (naphthalene)

Anthra- (anthracene)

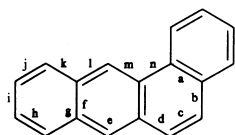
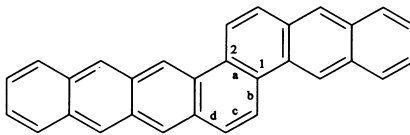
Perylo- (perylene)

Benzo- (benzene)

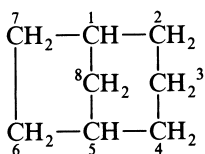
Phenanthro- (phenanthrene)

For monocyclic prefixes other than benzo-, the following names are recognized, each to represent the form with the maximum number of noncumulative double bonds: cyclopenta-, cyclohepta-, cycloocta-, etc.

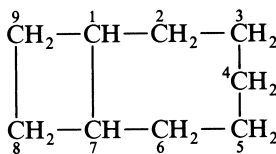
Isomers are distinguished by lettering the peripheral sides of the parent beginning with *a* for the side 1,2, and so on, lettering every side around the periphery. If necessary for clarity, the numbers of the attached position (1,2, for example) of the substituent ring are also denoted. The prefixes are cited in alphabetical order. The numbers and letters are enclosed in square brackets and placed immediately after the designation of the attached component. Examples are

Benz[ $\alpha$ ]anthraceneAnthra[2,1- $\alpha$ ]naphthacene

**1.1.1.6 Bridged Hydrocarbons.** Saturated alicyclic hydrocarbon systems consisting of two rings that have two or more atoms in common take the name of the open-chain hydrocarbon containing the same total number of carbon atoms and are preceded by the prefix bicyclo-. The system is numbered commencing with one of the bridgeheads, numbering proceeding by the longest possible path to the second bridgehead. Numbering is then continued from this atom by the longer remaining unnumbered path back to the first bridgehead and is completed by the shortest path from the atom next to the first bridgehead. When a choice in numbering exists, unsaturation is given the lowest numbers. The number of carbon atoms in each of the bridges connecting the bridgeheads is indicated in brackets in descending order. Examples are



Bicyclo[3.2.1]octane

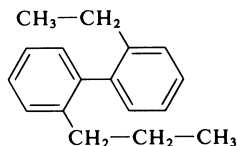


Bicyclo[5.2.0]nonane

**1.1.1.7 Hydrocarbon Ring Assemblies.** Assemblies are two or more cyclic systems, either single rings or fused systems, that are joined directly to each other by double or single bonds. For identical systems naming may proceed (1) by placing the prefix bi- before the name of the corresponding radical or (2), for systems joined through a single bond, by placing the prefix bi- before the name of the corresponding hydrocarbon. In each case, the numbering of the assembly is that of the corresponding radical or hydrocarbon, one system being assigned unprimed numbers and the other primed numbers. The points of attachment are indicated by placing the appropriate locants before the name; an unprimed number is considered lower than the same number primed. The name *biphenyl* is used for the assembly consisting of two benzene rings. Examples are



1,1'-Bicycloppropyl or 1,1'-bicyclopropane



2-Ethyl-2'-propylbiphenyl

For nonidentical ring systems, one ring system is selected as the parent and the other systems are considered as substituents and are arranged in alphabetical order. The parent ring system is assigned unprimed numbers. The parent is chosen by considering the following characteristics in turn until a decision is reached: (1) the system containing the larger number of rings, (2) the system containing the larger ring, (3) the system in the lowest state of hydrogenation, and (4) the highest-order number of ring systems set forth in Table 1.2. Examples are given, with the deciding priority given in parentheses preceding the name:

- (1) 2-Phenyl(naphthalene)
- (2) and (4) 2-(2'-Naphthyl)azulene
- (3) Cyclohexylbenzene

**1.1.1.8 Radicals from Ring Systems.** Univalent substituent groups derived from polycyclic hydrocarbons are named by changing the final *e* of the hydrocarbon name to -yl. The carbon atoms having free valences are given locants as low as possible consistent with the fixed numbering of the



hydrocarbon. Exceptions are naphthyl (instead of naphthalenyl), anthryl (for anthracenyl), and phenanthryl (for phenanthrenyl). However, these abbreviated forms are used only for the simple ring systems. Substituting groups derived from fused derivatives of these ring systems are named systematically. Substituting groups having two or more free bonds are named as described in Monocyclic Aliphatic Hydrocarbons on p. 1.5.

**1.1.1.9 Cyclic Hydrocarbons with Side Chains.** Hydrocarbons composed of cyclic and aliphatic chains are named in a manner that is the simplest permissible or the most appropriate for the chemical intent. Hydrocarbons containing several chains attached to one cyclic nucleus are generally named as derivatives of the cyclic compound, and compounds containing several side chains and/or cyclic radicals attached to one chain are named as derivatives of the acyclic compound. Examples are

2-Ethyl-1-methylnaphthalene

Diphenylmethane

1,5-Diphenylpentane

2,3-Dimethyl-1-phenyl-1-hexene

Recognized trivial names for composite radicals are used if they lead to simplifications in naming. Examples are

1-Benzyl-naphthalene

1,2,4-Tris(3-*p*-tolylpropyl)benzene

Fulvene, for methylenecyclopentadiene, and stilbene, for 1,2-diphenylethylene, are trivial names that are retained.

**1.1.1.10 Heterocyclic Systems.** Heterocyclic compounds can be named by relating them to the corresponding carbocyclic ring systems by using replacement nomenclature. Heteroatoms are denoted by prefixes ending in *a*, as shown in Table 1.3. If two or more replacement prefixes are required in a single name, they are cited in the order of their listing in the table. The lowest possible numbers consistent with the numbering of the corresponding carbocyclic system are assigned to the heteroatoms and then to carbon atoms bearing double or triple bonds. Locants are cited immediately preceding the prefixes or suffixes to which they refer. Multiplicity of the same heteroatom is indicated by the appropriate prefix in the series: di-, tri-, tetra-, penta-, hexa-, etc.

**TABLE 1.3** Specialist Nomenclature for Heterocyclic Systems

*Heterocyclic atoms are listed in decreasing order of priority.*

| Element    | Valence | Prefix    | Element   | Valence | Prefix   |
|------------|---------|-----------|-----------|---------|----------|
| Oxygen     | 2       | Oxa-      | Antimony  | 3       | Stiba-*  |
| Sulfur     | 2       | Thia-     | Bismuth   | 3       | Bisma-   |
| Selenium   | 2       | Selena-   | Silicon   | 4       | Sila-    |
| Tellurium  | 2       | Tellura-  | Germanium | 4       | Germa-   |
| Nitrogen   | 3       | Aza-      | Tin       | 4       | Stanna-  |
| Phosphorus | 3       | Phospha-* | Lead      | 4       | Plumba-  |
| Arsenic    | 3       | Arsa-*    | Boron     | 3       | Bora-    |
|            |         |           | Mercury   | 2       | Mercura- |

\* When immediately followed by -in or -ine, phospha- should be replaced by phosphor-, arsa- by arsen-, and stiba- by antimon-. The saturated six-membered rings corresponding to phosphorin and arsenin are named *phosphorinane* and *arsenane*. A further exception is the replacement of borin by borinane.

**TABLE 1.4** Suffixes for Specialist Nomenclature of Heterocyclic Systems

| Number of ring members | Rings containing nitrogen |            | Rings containing no nitrogen |            |
|------------------------|---------------------------|------------|------------------------------|------------|
|                        | Unsaturation*             | Saturation | Unsaturation*                | Saturation |
| 3                      | -irine                    | -iridine   | -irene                       | -irane     |
| 4                      | -ete                      | -etidine   | -ete                         | -etane     |
| 5                      | -ole                      | -olidine   | -ole                         | -olane     |
| 6                      | -ine†                     | ‡          | -in                          | -ane§      |
| 7                      | -epine                    | ‡          | -epin                        | -epane     |
| 8                      | -ocine                    | ‡          | -ocin                        | -ocane     |
| 9                      | -onine                    | ‡          | -onin                        | -onane     |
| 10                     | -ecine                    | ‡          | -ecin                        | -ecane     |

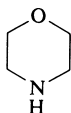
\* Unsaturation corresponding to the maximum number of noncumulative double bonds. Heteroatoms have the normal valences given in Table 1.3.

† For phosphorus, arsenic, antimony, and boron, see the special provisions in Table 1.3.

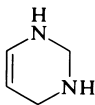
‡ Expressed by prefixing perhydro- to the name of the corresponding unsaturated compound.

§ Not applicable to silicon, germanium, tin, and lead; perhydro- is prefixed to the name of the corresponding unsaturated compound.

If the corresponding carbocyclic system is partially or completely hydrogenated, the additional hydrogen is cited using the appropriate *H*- or hydro- prefixes. A trivial name from Tables 1.5 and 1.6, if available, along with the state of hydrogenation may be used. In the specialist nomenclature for heterocyclic systems, the prefix or prefixes from Table 1.3 are combined with the appropriate stem from Table 1.4, eliding an *a* where necessary. Examples of acceptable usage, including (1) replacement and (2) specialist nomenclature, are



- (1) 1-Oxa-4-azacyclohexane  
(2) 1,4-Oxazoline  
Morpholine



- (1) 1,3-Diazacyclohex-5-ene  
(2) 1,2,3,4-Tetrahydro-1,3-diazine



- (1) Thiacyclopropane  
(2) Thiirane  
Ethylene sulfide

Radicals derived from heterocyclic compounds by removal of hydrogen from a ring are named by adding -yl to the names of the parent compounds (with elision of the final *e*, if present). These exceptions are retained:

Furyl (from furan)

Pyridyl (from pyridine)

Piperidyl (from piperidine)

Quinolyl (from quinoline)

Isoquinolyl

Thenylidene (for thienylmethylene)

Furfuryl (for 2-furylmethyl)

Furfurylidene (for 2-furylmethylene)

Thienyl (from thiophene)

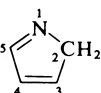
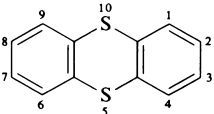
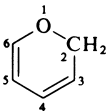
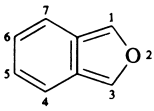
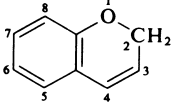
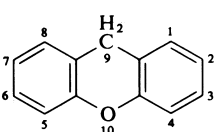
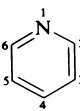
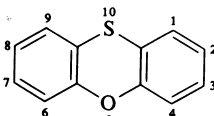
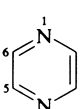
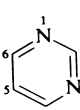
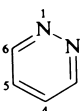
Thenylidyne (for thienylmethyldiyne)

Furfuryldiyne (for 2-furylmethyldiyne)

Thenyl (for thienylmethyl)

Also, piperidino- and morpholino- are preferred to 1-piperidyl- and 4-morpholinyl-, respectively.

**TABLE 1.5** Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names  
*Listed in order of increasing priority as senior ring system.*

| Structure                                                                          | Parent name            | Radical name    | Structure                                                                           | Parent name | Radical name |
|------------------------------------------------------------------------------------|------------------------|-----------------|-------------------------------------------------------------------------------------|-------------|--------------|
|    | Thiophene              | Thienyl         |    | 2H-Pyrrole  | 2H-Pyrrolyl  |
|    | Thianthrene            | Thianthrenyl    |    | Pyrrole     | Pyrrolyl     |
|    | Furan                  | Furyl           |    | Imidazole   | Imidazolyl   |
|    | Pyran<br>(2H-shown)    | Pyranyl         |    | Pyrazole    | Pyrazolyl    |
|    | Isobenzofuran          | Isobenzofuranyl |    | Isothiazole | Isothiazolyl |
|   | Chromene<br>(2H-shown) | Chromenyl       |    | Isoxazole   | Isoxazolyl   |
|  | Xanthene*              | Xanthenyl       |   | Pyridine    | Pyridyl      |
|  | Phenoxathiin           | Phenoxathiinyl  |  | Pyrazine    | Pyrazinyl    |
|                                                                                    |                        |                 |  | Pyrimidine  | Pyrimidinyl  |
|                                                                                    |                        |                 |  | Pyridazine  | Pyridazinyl  |

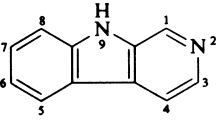
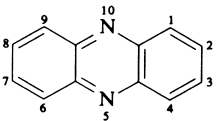
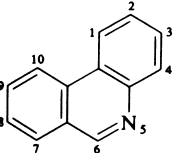
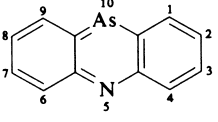
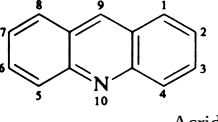
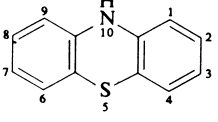
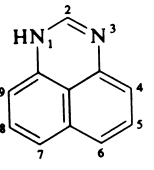
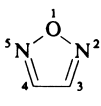
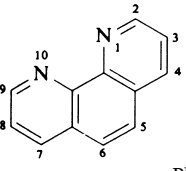
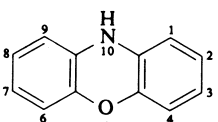
\* Asterisk after a compound denotes exception to systematic numbering.

**TABLE 1.5** Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (*Continued*)

| Structure | Parent name    | Radical name    | Structure | Parent name                  | Radical name   |
|-----------|----------------|-----------------|-----------|------------------------------|----------------|
|           | Indolizine     | IndolizinyI     |           | Phthalazine                  | Phthalazinyl   |
|           | Isoindole      | Isoindolyl      |           | Naphthyridine<br>(1,8-shown) | Naphthyridinyl |
|           | 3H-Indole      | 3H-Indolyl      |           | Quinoxaline                  | QuinoxalinyI   |
|           | Indole         | Indolyl         |           | Quinazoline                  | QuinazolinyI   |
|           | 1H-Indazole    | 1H-Indazolyl    |           | Cinnoline                    | CinnolinyI     |
|           | Purine*        | PurinyI         |           | Pteridine                    | Pteridinyl     |
|           | 4H-Quinolizine | 4H-QuinolizinyI |           | 4aH-Carbazole*               | 4aH-Carbazolyl |
|           | Isoquinoline   | Isoquinolyl     |           | Carbazole*                   | Carbazolyl     |
|           | Quinolone      | Quinolyl        |           |                              |                |

\* Asterisk after a compound denotes exception to systematic numbering.

**TABLE 1.5** Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (*Continued*)

| Structure                                                                         | Parent name                    | Radical name        | Structure                                                                           | Parent name   | Radical name   |
|-----------------------------------------------------------------------------------|--------------------------------|---------------------|-------------------------------------------------------------------------------------|---------------|----------------|
|   | $\beta$ -Carboline             | $\beta$ -Carbolinyl |    | Phenazine     | Phenazinyl     |
|   | Phenanthridine                 | Phenanthridinyl     |    | Phenarsazine  | Phenarsazinyl  |
|   | Acridine*                      | Acridinyl           |    | Phenothiazine | Phenothiazinyl |
|   | Perimidine                     | Perimidinyl         |    | Furazan       | Furazanyl      |
|  | Phenanthroline<br>(1,10-shown) | Phenanthrolinyl     |  | Phenoxazine   | Phenoxazinyl   |

\* Asterisk after a compound denotes exception to systematic numbering.

If there is a choice among heterocyclic systems, the parent compound is decided in the following order of preference:

1. A nitrogen-containing component
2. A component containing a heteroatom, in the absence of nitrogen, as high as possible in Table 1.3
3. A component containing the greater number of rings

**TABLE 1.6** Trivial Names of Heterocyclic Systems That Are Not Recommended for Use in Fusion Names  
Listed in order of increasing priority.

| Structure | Parent name               | Radical name   | Structure | Parent name              | Radical name  |
|-----------|---------------------------|----------------|-----------|--------------------------|---------------|
|           | Isochroman                | Isochromanyl   |           | Pyrazoline<br>(3-shown*) | Pyrazolinyl   |
|           | Chroman                   | Chromanyl      |           | Piperidine               | Piperidyl†    |
|           | Pyrrolidine               | Pyrrolinyl     |           | Piperazine               | Piperazinyl   |
|           | Pyrroline<br>(2-shown*)   | Pyrrolinyl     |           | Indoline                 | Indolinyl     |
|           | Imidazolidine             | Imidazolidinyl |           | Isoindoline              | Isoindolinyl  |
|           | Imidazoline<br>(2-shown*) | Imidazoliny    |           | Quinuclidine             | Quinuclidinyl |
|           | Pyrazolidine              | Pyrazolidinyl  |           | Morpholine               | Morpholinyl‡  |

\* Denotes position of double bond.

† For 1-piperidyl, use piperidino.

‡ For 4-morpholinyl, use morpholino.

- A component containing the largest possible individual ring
- A component containing the greatest number of heteroatoms of any kind
- A component containing the greatest variety of heteroatoms
- A component containing the greatest number of heteroatoms first listed in Table 1.3

If there is a choice between components of the same size containing the same number and kind of heteroatoms, choose as the base component that one with the lower numbers for the heteroatoms before fusion. When a fusion position is occupied by a heteroatom, the names of the component rings to be fused are selected to contain the heteroatom.

### 1.1.2 Functional Compounds

There are several types of nomenclature systems that are recognized. Which type to use is sometimes obvious from the nature of the compound. Substitutive nomenclature, in general, is preferred because of its broad applicability, but radicofunctional, additive, and replacement nomenclature systems are convenient in certain situations.

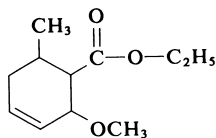
**1.1.2.1 Substitutive Nomenclature.** The first step is to determine the kind of characteristic (functional) group for use as the principal group of the parent compound. A characteristic group is a recognized combination of atoms that confers characteristic chemical properties on the molecule in which it occurs. Carbon-to-carbon unsaturation and heteroatoms in rings are considered nonfunctional for nomenclature purposes.

*Substitution* means the replacement of one or more hydrogen atoms in a given compound by some other kind of atom or group of atoms, functional or nonfunctional. In substitutive nomenclature, each substituent is cited as either a prefix or a suffix to the name of the parent (or substituting radical) to which it is attached; the latter is denoted the parent compound (or parent group if a radical).

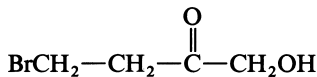
In Table 1.7 are listed the general classes of compounds in descending order of preference for citation as suffixes, that is, as the parent or characteristic compound. When oxygen is replaced by sulfur, selenium, or tellurium, the priority for these elements is in the descending order listed. The higher valence states of each element are listed before considering the successive lower valence states. Derivative groups have priority for citation as principal group after the respective parents of their general class.

In Table 1.8 are listed characteristic groups that are cited only as prefixes (never as suffixes) in substitutive nomenclature. The order of listing has no significance for nomenclature purposes.

Systematic names formed by applying the principles of substitutive nomenclature are single words except for compounds named as acids. First one selects the parent compound, and thus the suffix, from the characteristic group listed earliest in Table 1.7. All remaining functional groups are handled as prefixes that precede, in alphabetical order, the parent name. Two examples may be helpful:



Structure I



Structure II

Structure I contains an ester group and an ether group. Since the ester group has higher priority, the name is ethyl 2-methoxy-6-methyl-3-cyclohexene-1-carboxylate. Structure II contains a carbonyl group, a hydroxy group, and a bromo group. The latter is never a suffix. Between the other two, the carbonyl group has higher priority, the parent has -one as suffix, and the name is 4-bromo-1-hydroxy-2-butanone.

Selection of the principal alicyclic chain or ring system is governed by these selection rules:

1. For purely alicyclic compounds, the selection process proceeds successively until a decision is reached: (a) the maximum number of substituents corresponding to the characteristic group cited earliest in Table 1.7, (b) the maximum number of double and triple bonds considered together, (c) the maximum length of the chain, and (d) the maximum number of double bonds. Additional criteria, if needed for complicated compounds, are given in the IUPAC nomenclature rules.
2. If the characteristic group occurs only in a chain that carries a cyclic substituent, the compound is named as an aliphatic compound into which the cyclic component is substituted; a radical prefix is used to denote the cyclic component. This chain need not be the longest chain.
3. If the characteristic group occurs in more than one carbon chain and the chains are not directly

**TABLE 1.7** Characteristic Groups for Substitutive Nomenclature

Listed in order of decreasing priority for citation as principal group or parent name.

| Class                    | Formula*                                                                                                                                                                              | Prefix                                                                                          | Suffix                                                                                                 |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
| 1. Cations:              | $\text{H}_4\text{N}^+$<br>$\text{H}_3\text{O}^+$<br>$\text{H}_3\text{S}^+$<br>$\text{H}_3\text{Se}^+$<br>$\text{H}_2\text{Cl}^+$<br>$\text{H}_2\text{Br}^+$<br>$\text{H}_2\text{I}^+$ | -onio-<br>Ammonio-<br>Oxonio-<br>Sulfonio-<br>Selenonio-<br>Chloronio-<br>Bromonio-<br>Iodonio- | -onium<br>-ammonium<br>-oxonium<br>-sulfonium<br>-selenonium<br>-chloronium<br>-bromonium<br>-iodonium |
| 2. Acids:                |                                                                                                                                                                                       |                                                                                                 |                                                                                                        |
| Carboxylic               | $-\text{COOH}$<br>$-(\text{C})\text{OOH}$<br>$-\text{C}(=\text{O})\text{OOH}$                                                                                                         | Carboxy-                                                                                        | -carboxylic acid<br>-oic acid<br>-peroxy···carboxylic acid<br>-peroxy···oic acid                       |
| Sulfonic                 | $-\text{SO}_3\text{H}$                                                                                                                                                                | Sulfo-                                                                                          | -sulfonic acid                                                                                         |
| Sulfinic                 | $-\text{SO}_2\text{H}$                                                                                                                                                                | Sulfino-                                                                                        | -sulfinic acid                                                                                         |
| Sulfenic                 | $-\text{SOH}$                                                                                                                                                                         | Sulfeno-                                                                                        | -sulfenic acid                                                                                         |
| Salts                    | $-\text{COOM}$<br>$-(\text{C})\text{OOM}$<br>$-\text{SO}_3\text{M}$<br>$-\text{SO}_2\text{M}$<br>$-\text{SOM}$                                                                        |                                                                                                 | Metal···carboxylate<br>Metal···oate<br>Metal···sulfonate<br>Metal···sulfinate<br>Metal···sulfenate     |
| 3. Derivatives of acids: |                                                                                                                                                                                       |                                                                                                 |                                                                                                        |
| Anhydrides               | $-\text{C}(=\text{O})\text{OC}(=\text{O})-$<br>$-(\text{C}=\text{O})\text{O}(\text{C}=\text{O})-$                                                                                     |                                                                                                 | -carboxylic anhydride<br>-oic anhydride                                                                |
| Esters                   | $-\text{COOR}$<br>$-\text{C}(\text{OOR})$                                                                                                                                             | R-oxycarbonyl-                                                                                  | R···carboxylate<br>R···oate                                                                            |
| Acid halides             | $-\text{CO}-\text{halogen}$                                                                                                                                                           | Haloformyl                                                                                      | -carbonyl halide                                                                                       |
| Amides                   | $-\text{CO}-\text{NH}_2$<br>$(\text{C})\text{O}-\text{NH}_2$                                                                                                                          | Carbamoyl-                                                                                      | -carboxamide<br>-amide                                                                                 |



**TABLE 1.7** Characteristic Groups for Substitutive Nomenclature (*Continued*)

| Class                        | Formula*                             | Prefix                  | Suffix          |
|------------------------------|--------------------------------------|-------------------------|-----------------|
| Hydrazides                   | $\text{—CO—NHNH}_2$                  | Carbonyl-<br>hydrazino- | -carbohydrazide |
| Imides                       | $\text{—(CO)—NHNH}_2$                |                         | -ohydrazide     |
| Amidines                     | $\text{—CO—NH—CO—}$                  | R-imido-                | -carboximide    |
|                              | $\text{—C(=NH)—NH}_2$                | Amidino-                | -carboxamidine  |
|                              | $\text{—(C=NH)—NH}_2$                |                         | -amidine        |
| 4. Nitrile (cyanide)         | $\text{—CN}$                         | Cyano-                  | -carbonitrile   |
|                              | $\text{—(C)N}$                       |                         | -nitrile        |
| 5. Aldehydes                 | $\text{—CHO}$                        | Formyl-                 | -carbaldehyde   |
|                              | $\text{—(C=O)H}$                     | Oxo-                    | -al             |
|                              | (then their analogs and derivatives) |                         |                 |
| 6. Ketones                   | $\text{>(C=O)}$                      | Oxo-                    | -one            |
|                              | (then their analogs and derivatives) |                         |                 |
| 7. Alcohols<br>(and phenols) | $\text{—OH}$                         | Hydroxy-                | -ol             |
| Thiols                       | $\text{—SH}$                         | Mercapto-               | -thiol          |
| 8. Hydroperoxides            | $\text{—O—OH}$                       | Hydroperoxy-            |                 |
| 9. Amines                    | $\text{—NH}_2$                       | Amino-                  | -amine          |
| Imines                       | $\text{>NH}$                         | Imino-                  | -imine          |
| Hydrazines                   | $\text{—NHNH}_2$                     | Hydrazino-              | -hydrazine      |
| 10. Ethers                   | $\text{—OR}$                         | R-oxy-                  |                 |
| Sulfides                     | $\text{—SR}$                         | R-thio-                 |                 |
| 11. Peroxides                | $\text{—O—OR}$                       | R-dioxy-                |                 |

\* Carbon atoms enclosed in parentheses are included in the name of the parent compound and not in the suffix or prefix.

**TABLE 1.8** Characteristic Groups Cited Only as Prefixes in Substitutive Nomenclature

| Characteristic group | Prefix         | Characteristic group | Prefix                                                                                                   |
|----------------------|----------------|----------------------|----------------------------------------------------------------------------------------------------------|
| $\text{—Br}$         | Bromo-         | $\text{—IX}_2$       | X may be halogen or a radical; dihalogenoiodo- or diacetoxyiodo-, e.g., $\text{—ICl}_2$ is dichloroiodo- |
| $\text{—Cl}$         | Chloro-        |                      |                                                                                                          |
| $\text{—ClO}$        | Chlorosyl-     | $\text{>N}_2$        | Diazo-                                                                                                   |
| $\text{—ClO}_2$      | Chloryl-       | $\text{—N}_3$        | Azido-                                                                                                   |
| $\text{—ClO}_3$      | Perchloryl-    | $\text{—NO}$         | Nitroso-                                                                                                 |
| $\text{—F}$          | Fluoro-        | $\text{—NO}_2$       | Nitro-                                                                                                   |
| $\text{—I}$          | Iodo-          | $\text{>N(=O)OH}$    | <i>aci</i> -Nitro-                                                                                       |
| $\text{—IO}$         | Iodosyl-       | $\text{—OR}$         | R-oxy-                                                                                                   |
| $\text{—IO}_2$       | Iodyl*         | $\text{—SR}$         | R-thio-                                                                                                  |
| $\text{—I(OH)}_2$    | Dihydroxyiodo- | $\text{—SeR (—TeR)}$ | R-seleno- (R-telluro-)                                                                                   |

\* Formerly iodoxy.

attached to one another, then the chain chosen as parent should carry the largest number of the characteristic group. If necessary, the selection is continued as in rule 1.

4. If the characteristic group occurs only in one cyclic system, that system is chosen as the parent.
5. If the characteristic group occurs in more than one cyclic system, that system is chosen as parent which (a) carries the largest number of the principal group or, failing to reach a decision, (b) is the senior ring system.
6. If the characteristic group occurs both in a chain and in a cyclic system, the parent is that portion in which the principal group occurs in largest number. If the numbers are the same, that portion is chosen which is considered to be the most important or is the senior ring system.
7. When a substituent is itself substituted, all the subsidiary substituents are named as prefixes and the entire assembly is regarded as a parent radical.
8. The seniority of ring systems is ascertained by applying the following rules successively until a decision is reached: (a) all heterocycles are senior to all carbocycles, (b) for heterocycles, the preference follows the decision process described under Heterocyclic Systems, p. 1.11, (c) the largest number of rings, (d) the largest individual ring at the first point of difference, (e) the largest number of atoms in common among rings, (f) the lowest letters in the expression for ring functions, (g) the lowest numbers at the first point of difference in the expression for ring junctions, (h) the lowest state of hydrogenation, (i) the lowest-numbered locant for indicated hydrogen, (j) the lowest-numbered locant for point of attachment (if a radical), (k) the lowest-numbered locant for an attached group expressed as a suffix, (l) the maximum number of substituents cited as prefixes, (m) the lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order independent of their nature, and (n) the lowest-numbered locant for the substituent named as prefix which is cited first in the name.

*Numbering of Compounds.* If the rules for aliphatic chains and ring systems leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest-numbered locants to these structural factors, if present, considered successively in the order listed below until a decision is reached. Characteristic groups take precedence over multiple bonds.

1. Indicated hydrogen, whether cited in the name or omitted as being conventional
2. Characteristic groups named as suffix following the ranking order of Table 1.7
3. Multiple bonds in acyclic compounds; in bicycloalkanes, tricycloalkanes, and polycycloalkanes, double bonds having priority over triple bonds; and in heterocyclic systems whose names end in -etine, -oline, or -olene
4. The lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order
5. The lowest locant for that substituent named as prefix which is cited first in the name

For cyclic radicals, indicated hydrogen and thereafter the point of attachment (free valency) have priority for the lowest available number.

*Prefixes and Affixes.* Prefixes are arranged alphabetically and placed before the parent name; multiplying affixes, if necessary, are inserted and *do not* alter the alphabetical order already attained. The parent name includes any syllables denoting a change of ring member or relating to the structure of a carbon chain. Nondetachable parts of parent names include

1. Forming rings; cyclo-, bicyclo-, spiro-
2. Fusing two or more rings: benzo-, naphtho-, imidazo-
3. Substituting one ring or chain member atom for another: oxa-, aza-, thia-
4. Changing positions of ring or chain members: iso-, *sec*-, *tert*-, neo-
5. Showing indicated hydrogen
6. Forming bridges: ethano-, epoxy-
7. Hydro-

Prefixes that represent complete terminal characteristic groups are preferred to those representing only a portion of a given group. For example, for the prefix  $\text{—C(=O)CH}_3$ , the name (formylmethyl) is preferred to (oxoethyl).

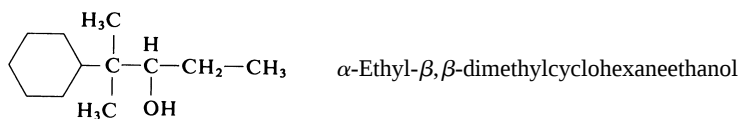
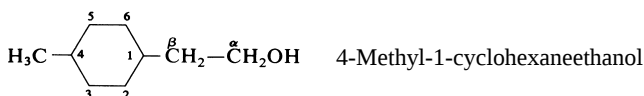
The multiplying affixes di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-, undeca-, and so on are used to indicate a set of *identical* unsubstituted radicals or parent compounds. The forms bis-, tris-, tetrakis-, pentakis-, and so on are used to indicate a set of identical radicals or parent compounds *each substituted in the same way*. The affixes bi-, ter-, quater-, quinque-, sexi-, septi-, octi-, novi-, deci-, and so on are used to indicate the number of identical rings joined together by a single or double bond.

Although multiplying affixes may be omitted for very common compounds when no ambiguity is caused thereby, such affixes are generally included throughout this handbook in alphabetical listings. An example would be ethyl ether for diethyl ether.

**1.1.2.2 Conjunctive Nomenclature.** Conjunctive nomenclature may be applied when a principal group is attached to an acyclic component that is directly attached by a carbon-carbon bond to a cyclic component. The name of the cyclic component is attached directly in front of the name of the acyclic component carrying the principal group. This nomenclature is not used when an unsaturated side chain is named systematically. When necessary, the position of the side chain is indicated by a locant placed before the name of the cyclic component. For substituents on the acyclic chain, carbon atoms of the side chain are indicated by Greek letters proceeding from the principal group to the cyclic component. The terminal carbon atom of acids, aldehydes, and nitriles is omitted when allocating Greek positional letters. Conjunctive nomenclature is not used when the side chain carries more than one of the principal group, except in the case of malonic and succinic acids.

The side chain is considered to extend only from the principal group to the cyclic component. Any other chain members are named as substituents, with appropriate prefixes placed before the name of the cyclic component.

When a cyclic component carries more than one identical side chain, the name of the cyclic component is followed by di-, tri-, etc., and then by the name of the acyclic component, and it is preceded by the locants for the side chains. Examples are



When side chains of two or more different kinds are attached to a cyclic component, only the senior side chain is named by the conjunctive method. The remaining side chains are named as prefixes. Likewise, when there is a choice of cyclic component, the senior is chosen. Benzene derivatives may be named by the conjunctive method only when two or more identical side chains are present. Trivial names for oxo carboxylic acids may be used for the acyclic component. If the cyclic and acyclic components are joined by a double bond, the locants of this bond are placed as superscripts to a Greek capital delta that is inserted between the two names. The locant for the cyclic component precedes that for the acyclic component, e.g., indene- $\Delta^{1,\alpha}$ -acetic acid.

**1.1.2.3 Radicofunctional Nomenclature.** The procedures of radicofunctional nomenclature are identical with those of substitutive nomenclature except that suffixes are never used. Instead, the functional class name (Table 1.9) of the compound is expressed as one word and the remainder of the molecule as another that precedes the class name. When the functional class name refers to a characteristic group that is bivalent, the two radicals attached to it are each named, and when different, they are written as separate words arranged in alphabetical order. When a compound contains more than one kind of group listed in Table 1.9, that kind is cited as the functional group or class name that occurs higher in the table, all others being expressed as prefixes.

Radicofunctional nomenclature finds some use in naming ethers, sulfides, sulfoxides, sulfones, selenium analogs of the preceding three sulfur compounds, and azides.

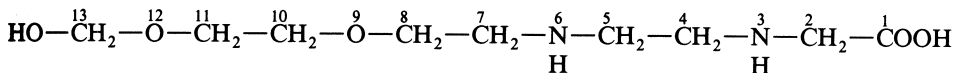
**TABLE 1.9** Functional Class Names Used in Radicofunctional Nomenclature

*Groups are listed in order of decreasing priority.*

| Group                        | Functional class names                                                                                                   |
|------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| X in acid derivatives        | Name of X (in priority order: fluoride, chloride, bromide, iodide, cyanide, azide; then the sulfur and selenium analogs) |
| —CN, —NC                     | Cyanide, isocyanide                                                                                                      |
| >CO                          | Ketone; then S and Se analogs                                                                                            |
| —OH                          | Alcohol; then S and Se analogs                                                                                           |
| —O—OH                        | Hydroperoxide                                                                                                            |
| >O                           | Ether or oxide                                                                                                           |
| >S, >SO, >SO <sub>2</sub>    | Sulfide, sulfoxide, sulfone                                                                                              |
| >Se, >SeO, >SeO <sub>2</sub> | Selenide, selenoxide, selenone                                                                                           |
| —F, —Cl, —Br, —I             | Fluoride, chloride, bromide, iodide                                                                                      |
| —N <sub>3</sub>              | Azide                                                                                                                    |

**1.1.2.4 Replacement Nomenclature.** Replacement nomenclature is intended for use only when other nomenclature systems are difficult to apply in the naming of chains containing heteroatoms. When no group is present that can be named as a principal group, the longest chain of carbon and heteroatoms terminating with carbon is chosen and named as though the entire chain were that of an acyclic hydrocarbon. The heteroatoms within this chain are identified by means of prefixes aza-, oxa-, thia-, etc., in the order of priority stated in Table 1.3. Locants indicate the positions of the heteroatoms in the chain. Lowest-numbered locants are assigned to the principal group when

such is present. Otherwise, lowest-numbered locants are assigned to the heteroatoms considered together and, if there is a choice, to the heteroatoms cited earliest in Table 1.3. An example is



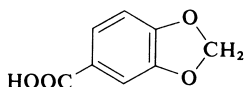
13-Hydroxy-9,12-dioxa-3,6-diazatridecanoic acid

### 1.1.3 Specific Functional Groups

Characteristic groups will now be treated briefly in order to expand the terse outline of substitutive nomenclature presented in Table 1.7. Alternative nomenclature will be indicated whenever desirable.

**1.1.3.1 Acetals and Acylals.** Acetals, which contain the group  $>\text{C}(\text{OR})_2$ , where R may be different, are named (1) as dialkoxo compounds or (2) by the name of the corresponding aldehyde or ketone followed by the name of the hydrocarbon radical(s) followed by the word *acetal*. For example,  $\text{CH}_3-\text{CH}(\text{OCH}_3)_2$  is named either (1) 1,1-dimethoxyethane or (2) acetaldehyde dimethyl acetal.

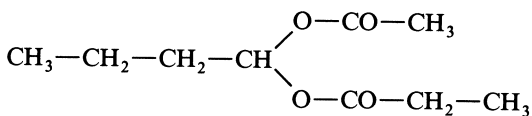
A cyclic acetal in which the two acetal oxygen atoms form part of a ring may be named (1) as a heterocyclic compound or (2) by use of the prefix methylenedioxy for the group  $-\text{O}-\text{CH}_2-\text{O}-$  as a substituent in the remainder of the molecule. For example,



(1) 1,3-Benzo[d]dioxole-5-carboxylic acid

(2) 3,4-Methylenedioxybenzoic acid

Acylals,  $\text{R}^1\text{R}^2\text{C}(\text{OCOR}^3)_2$ , are named as acid esters;



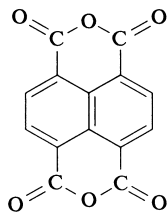
Butylidene acetate  
propionate

$\alpha$ -Hydroxy ketones, formerly called acyloins, had been named by changing the ending -ic acid or -oic acid of the corresponding acid to -oin. They are preferably named by substitutive nomenclature; thus



**1.1.3.2 Acid Anhydrides.** Symmetrical anhydrides of monocarboxylic acids, when unsubstituted, are named by replacing the word *acid* by *anhydride*. Anhydrides of substituted monocarboxylic acids, if symmetrically substituted, are named by prefixing bis- to the name of the acid and replacing the word *acid* by *anhydride*. Mixed anhydrides are named by giving in alphabetical order the first part of the names of the two acids followed by the word *anhydride*, e.g., acetic propionic anhydride or acetic propanoic anhydride. Cyclic anhydrides of polycarboxylic acids, although possessing a

heterocyclic structure, are preferably named as acid anhydrides. For example,



1,8;4,5-Naphthalenetetracarboxylic dianhydride (note the use of a semicolon to distinguish the pairs of locants)

**1.1.3.3 Acyl Halides.** Acyl halides, in which the hydroxyl portion of a carboxyl group is replaced by a halogen, are named by placing the name of the corresponding halide after that of the acyl radical. When another group is present that has priority for citation as principal group or when the acyl halide is attached to a side chain, the prefix haloformyl- is used as, for example, in fluoroformyl-.

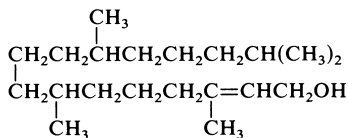
**1.1.3.4 Alcohols and Phenols.** The hydroxyl group is indicated by a suffix -ol when it is the principal group attached to the parent compound and by the prefix hydroxy- when another group with higher priority for citation is present or when the hydroxy group is present in a side chain. When confusion may arise in employing the suffix -ol, the hydroxy group is indicated as a prefix; this terminology is also used when the hydroxyl group is attached to a heterocycle, as, for example, in the name 3-hydroxythiophene to avoid confusion with thiophenol ( $\text{C}_6\text{H}_5\text{SH}$ ). Designations such as isopropanol, *sec*-butanol, and *tert*-butanol are incorrect because no hydrocarbon exists to which the suffix can be added. Many trivial names are retained. These structures are shown in Table 1.10. The radicals ( $\text{RO}-$ ) are named by adding -oxy as a suffix to the name of the R radical, e.g., pentyloxy for  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{O}-$ . These contractions are exceptions: methoxy ( $\text{CH}_3\text{O}-$ ), ethoxy ( $\text{C}_2\text{H}_5\text{O}-$ ), propoxy ( $\text{C}_3\text{H}_7\text{O}-$ ), butoxy ( $\text{C}_4\text{H}_9\text{O}-$ ), and phenoxy ( $\text{C}_6\text{H}_5\text{O}-$ ). For unsubstituted radicals only, one may use isopropoxy [ $(\text{CH}_3)_2\text{CH}-\text{O}-$ ], isobutoxy [ $(\text{CH}_3)_2\text{CH}_2\text{CH}-\text{O}-$ ], *sec*-butoxy [ $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-\text{O}-$ ], and *tert*-butoxy [ $(\text{CH}_3)_3\text{C}-\text{O}-$ ].

**TABLE 1.10** Retained Trivial Names of Alcohols and Phenols with Structures

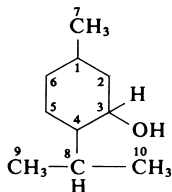
|                            |                                                                                                                                                                                                                          |
|----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ally alcohol               | $\text{CH}_2=\text{CHCH}_2\text{OH}$                                                                                                                                                                                     |
| <i>tert</i> -Butyl alcohol | $(\text{CH}_3)_3\text{COH}$                                                                                                                                                                                              |
| Benzyl alcohol             | $\text{C}_6\text{H}_5\text{CH}_2\text{OH}$                                                                                                                                                                               |
| Phenethyl alcohol          | $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{OH}$                                                                                                                                                                    |
| Ethylene glycol            | $\text{HOCH}_2\text{CH}_2\text{OH}$                                                                                                                                                                                      |
| 1,2-Propylene glycol       | $\text{CH}_3\text{CHOHCH}_2\text{OH}$                                                                                                                                                                                    |
| Glycerol                   | $\text{HOCH}_2\text{CHOHCH}_2\text{OH}$                                                                                                                                                                                  |
| Pentaerythritol            | $\text{C}(\text{CH}_2\text{OH})_4$                                                                                                                                                                                       |
| Pinacol                    | $(\text{CH}_3)_2\text{COHCOH}(\text{CH}_3)_2$                                                                                                                                                                            |
| Phenol                     | $\text{C}_6\text{H}_5\text{OH}$                                                                                                                                                                                          |
| Xylitol                    | $\begin{array}{ccccccc} & & \text{OH} & & & & \\ & &   & & & & \\ \text{HOCH}_2 & -\text{CH} & - & \text{CH} & - & \text{CH} & - \text{CH}_2\text{OH} \\ &   & & &   & & \\ & \text{OH} & & & \text{OH} & & \end{array}$ |
| Geraniol                   | $\begin{array}{c} (\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_2\text{C}=\text{CHCH}_2\text{OH} \\   \\ \text{CH}_3 \end{array}$                                                                                       |

**TABLE 1.10** Retained Trivial Names of Alcohols and Phenols with Structures (*Continued*)

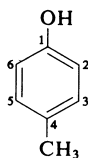
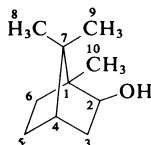
Phytol



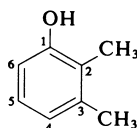
Menthol



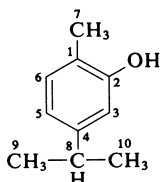
Borneol



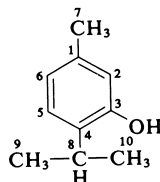
Cresol (1,4-isomer shown)



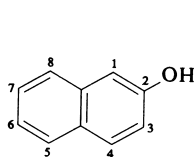
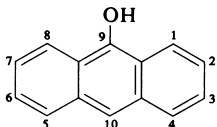
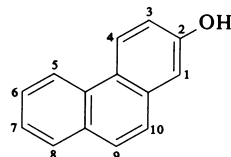
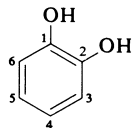
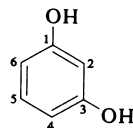
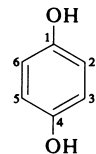
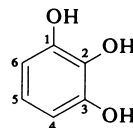
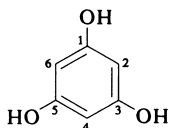
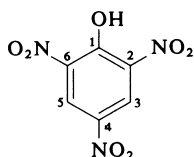
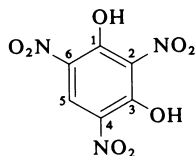
Xylenol (2,3-isomer shown)



Carvacrol



Thymol

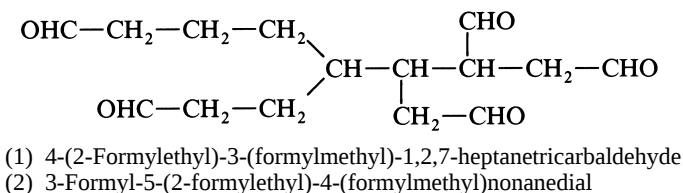
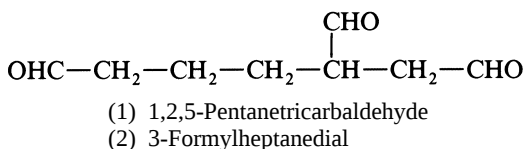
Naphthol (2-isomer shown)  
2-HydroxynaphthaleneAnthrol (9-isomer shown)  
9-HydroxyanthracenePhenanthrol (2-isomer shown)  
2-HydroxyphenanthrenePyrocatechol  
1,2-DihydroxybenzeneResorcinol  
1,3-DihydroxybenzeneHydroquinone  
1,4-DihydroxybenzenePyrogallol  
1,2,3-TrihydroxybenzenePhloroglucinol  
1,3,5-TrihydroxybenzenePicric acid  
2,4,6-TrinitrophenolStyphnic acid  
1,3-Dihydroxy-2,4,6-trinitrobenzene

Bivalent radicals of the form  $\text{O}-\text{Y}-\text{O}$  are named by adding -dioxy to the name of the bivalent radicals except when forming part of a ring system. Examples are  $-\text{O}-\text{CH}_2-\text{O}-$  (methylenedioxy),  $-\text{O}-\text{CO}-\text{O}-$  (carbonyldioxy), and  $-\text{O}-\text{SO}_2-\text{O}-$  (sulfonyldioxy). Anions derived from alcohols or phenols are named by changing the final -ol to -olate.

Salts composed of an anion,  $\text{RO}-$ , and a cation, usually a metal, can be named by citing first the cation and then the  $\text{RO}$  anion (with its ending changed to -yl oxide), e.g., sodium benzyl oxide for  $\text{C}_6\text{H}_5\text{CH}_2\text{ONa}$ . However, when the radical has an abbreviated name, such as methoxy, the ending -oxy is changed to -oxide. For example,  $\text{CH}_3\text{ONa}$  is named sodium methoxide (not sodium methylate).

**1.1.3.5 Aldehydes.** When the group  $-\text{C}(=\text{O})\text{H}$ , usually written  $-\text{CHO}$ , is attached to carbon at one (or both) end(s) of a linear acyclic chain the name is formed by adding the suffix -al (or -dial) to the name of the hydrocarbon containing the same number of carbon atoms. Examples are butanal for  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$  and propanedial for,  $\text{OHCCH}_2\text{CHO}$ .

Naming an acyclic polyaldehyde can be handled in two ways. First, when more than two aldehyde groups are attached to an unbranched chain, the proper affix is added to -carbaldehyde, which becomes the suffix to the name of the longest chain carrying the maximum number of aldehyde groups. The name and numbering of the main chain do not include the carbon atoms of the aldehyde groups. Second, the name is formed by adding the prefix formyl- to the name of the -dial that incorporates the principal chain. Any other chains carrying aldehyde groups are named by the use of formylalkyl- prefixes. Examples are



When the aldehyde group is directly attached to a carbon atom of a ring system, the suffix -carbaldehyde is added to the name of the ring system, e.g., 2-naphthalenecarbaldehyde. When the aldehyde group is separated from the ring by a chain of carbon atoms, the compound is named (1) as a derivative of the acyclic system or (2) by conjunctive nomenclature, for example, (1) (2-naphthyl)propionaldehyde or (2) 2-naphthalenepropionaldehyde.

An aldehyde group is denoted by the prefix formyl- when it is attached to a nitrogen atom in a ring system or when a group having priority for citation as principal group is present and part of a cyclic system.

When the corresponding monobasic acid has a trivial name, the name of the aldehyde may be formed by changing the ending -ic acid or -oic acid to -aldehyde. Examples are

|                 |                              |
|-----------------|------------------------------|
| Formaldehyde    | Acrylaldehyde (not acrolein) |
| Acetaldehyde    | Benzaldehyde                 |
| Propionaldehyde | Cinnamaldehyde               |
| Butyraldehyde   | 2-Furaldehyde (not furfural) |



The same is true for polybasic acids, with the proviso that all the carboxyl groups must be changed to aldehyde; then it is not necessary to introduce affixes. Examples are

Glyceraldehyde

Succinaldehyde

Glycolaldehyde

Phthalaldehyde (*o*-, *m*-, *p*-)

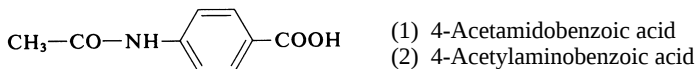
Malonaldehyde

These trivial names may be retained: citral (3,7-dimethyl-2,6-octadienal), vanillin (4-hydroxy-3-methoxybenzaldehyde), and piperonal (3,4-methylenedioxybenzaldehyde).

**1.1.3.6 Amides.** For primary amides the suffix -amide is added to the systematic name of the parent acid. For example,  $\text{CH}_3\text{—CO—NH}_2$  is acetamide. Oxamide is retained for  $\text{H}_2\text{N—CO—CO—NH}_2$ . The name -carboxylic acid is replaced by -carboxamide.

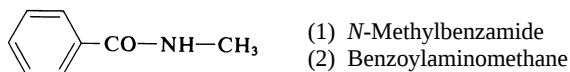
For amino acids having trivial names ending in -ine, the suffix -amide is added after the name of the acid (with elision of *e* for monoamides). For example,  $\text{H}_2\text{N—CH}_2\text{—CO—NH}_2$  is glycine-amide.

In naming the radical  $\text{R—CO—NH—}$ , either (1) the -yl ending of  $\text{RCO—}$  is changed to -amido or (2) the radicals are named as acylamino radicals. For example,

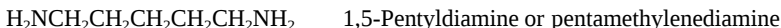


The latter nomenclature is always used for amino acids with trivial names.

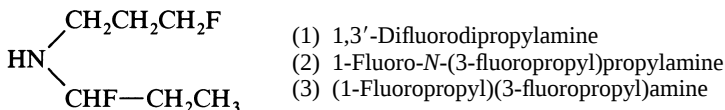
*N*-substituted primary amides are named either (1) by citing the substituents as *N* prefixes or (2) by naming the acyl group as an *N* substituent of the parent compound. For example,



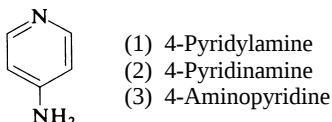
**1.1.3.7 Amines.** Amines are preferably named by adding the suffix -amine (and any multiplying affix) to the name of the parent radical. Examples are



Locants of substituents of symmetrically substituted derivatives of symmetrical amines are distinguished by primes or else the names of the complete substituted radicals are enclosed in parentheses. Unsymmetrically substituted derivatives are named similarly or as *N*-substituted products of a primary amine (after choosing the most senior of the radicals to be the parent amine). For example,



Complex cyclic compounds may be named by adding the suffix -amine or the prefix amino- (or aminoalkyl-) to the name of the parent compound. Thus three names are permissible for

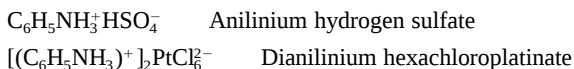


Complex linear polyamines are best designated by replacement nomenclature. These trivial names are retained: aniline, benzidine, phenetidine, toluidine, and xylydine.

The bivalent radical  $\text{—NH—}$  linked to two identical radicals can be denoted by the prefix imino-, as well as when it forms a bridge between two carbon ring atoms. A trivalent nitrogen atom linked to three identical radicals is denoted by the prefix nitrilo-. Thus ethylenediaminetetraacetic acid (an allowed exception) should be named ethylenedinitrilotetraacetic acid.

**1.1.3.8 Ammonium Compounds.** Salts and hydroxides containing quadricovalent nitrogen are named as a substituted ammonium salt or hydroxide. The names of the substituting radicals precede the word *ammonium*, and then the name of the anion is added as a separate word. For example,  $(\text{CH}_3)_4\text{N}^+\text{I}^-$  is tetramethylammonium iodide.

When the compound can be considered as derived from a base whose name does not end in -amine, its quaternary nature is denoted by adding ium to the name of that base (with elision of *e*), substituent groups are cited as prefixes, and the name of the anion is added separately at the end. Examples are



The names *choline* and *betaine* are retained for unsubstituted compounds.

In complex cases, the prefixes amino- and imino- may be changed to ammonio- and iminio- and are followed by the name of the molecule representing the most complex group attached to this nitrogen atom and are preceded by the names of the other radicals attached to this nitrogen. Finally the name of the anion is added separately. For example, the name might be 1-trimethylammonio-acridine chloride or 1-acridinyltrimethylammonium chloride.

When the preceding rules lead to inconvenient names, then (1) the unaltered name of the base may be used followed by the name of the anion or (2) for salts of hydrohalogen acids only the unaltered name of the base is used followed by the name of the hydrohalide. An example of the latter would be 2-ethyl-*p*-phenylenediamine monohydrochloride.

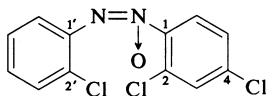
**1.1.3.9 Azo Compounds.** When the azo group ( $\text{—N=N—}$ ) connects radicals derived from identical unsubstituted molecules, the name is formed by adding the prefix azo- to the name of the parent unsubstituted molecules. Substituents are denoted by prefixes and suffixes. The azo group has priority for lowest-numbered locant. Examples are azobenzene for  $\text{C}_6\text{H}_5\text{—N=N—C}_6\text{H}_5$ , azobenzene-4-sulfonic acid for  $\text{C}_6\text{H}_5\text{—N=N—C}_6\text{H}_4\text{SO}_3\text{H}$ , and 2',4-dichloroazobenzene-4'-sulfonic acid for  $\text{ClC}_6\text{H}_4\text{—N=N—C}_6\text{H}_3\text{ClSO}_3\text{H}$ .

When the parent molecules connected by the azo group are different, azo is placed between the complete names of the parent molecules, substituted or unsubstituted. Locants are placed between the affix azo and the names of the molecules to which each refers. Preference is given to the more complex parent molecule for citation as the first component, e.g., 2-aminonaphthalene-1-azo-(4'-chloro-2'-methylbenzene).

In an alternative method, the senior component is regarded as substituted by  $\text{RN=N—}$ , this group R being named as a radical. Thus 2-(7-phenylazo-2-naphthylazo)anthracene is the name by this alternative method for the compound named anthracene-2-azo-2'-naphthalene-7'-azobenzene.

**1.1.3.10 Azoxy Compounds.** Where the position of the azoxy oxygen atom is unknown or immaterial, the compound is named in accordance with azo rules, with the affix azo replaced by azoxy. When the position of the azoxy oxygen atom in an unsymmetrical compound is designated, a prefix *NNO-* or *ONN-* is used. When both the groups attached to the azoxy radical are cited in the name of the compound, the prefix *NNO-* specifies that the second of these two groups is attached directly

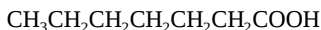
to  $\text{—N(O)—}$ ; the prefix *ONN-* specifies that the first of these two groups is attached directly to  $\text{—N(O)—}$ . When only one parent compound is cited in the name, the prefixed *ONN-* and *NNO-* specify that the group carrying the primed and unprimed substituents is connected, respectively, to the  $\text{—N(O)—}$  group. The prefix *NON-* signifies that the position of the oxygen atom is unknown; the azoxy group is then written as  $\text{—N}_2\text{O—}$ . For example,

2,2',4-Trichloro-*NNO*-azoxybenzene

**1.1.3.11 Boron Compounds.** Molecular hydrides of boron are called boranes. They are named by using a multiplying affix to designate the number of boron atoms and adding an Arabic numeral within parentheses as a suffix to denote the number of hydrogen atoms present. Examples are pentaborane(9) for  $\text{B}_5\text{H}_9$  and pentaborane(11) for  $\text{B}_5\text{H}_{11}$ .

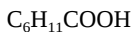
Organic ring systems are named by replacement nomenclature. Three- to ten-membered monocyclic ring systems containing uncharged boron atoms may be named by the specialist nomenclature for heterocyclic systems. Organic derivatives are named as outlined for substitutive nomenclature. The complexity of boron nomenclature precludes additional details; the text by Rigaudy and Klesney should be consulted.

**1.1.3.12 Carboxylic Acids.** Carboxylic acids may be named in several ways. First,  $\text{—COOH}$  groups replacing  $\text{CH}_3\text{—}$  at the end of the main chain of an acyclic hydrocarbon are denoted by adding -oic acid to the name of the hydrocarbon. Second, when the  $\text{—COOH}$  group is the principal group, the suffix -carboxylic acid can be added to the name of the parent chain whose name and chain numbering *does not include* the carbon atom of the  $\text{—COOH}$  group. The former nomenclature is preferred unless use of the ending -carboxylic acid leads to citation of a larger number of carboxyl groups as suffix. Third, carboxyl groups are designated by the prefix carboxy- when attached to a group named as a substituent or when another group is present that has higher priority for citation as principal group. In all cases, the principal chain should be linked to as many carboxyl groups as possible even though it might not be the longest chain present. Examples are

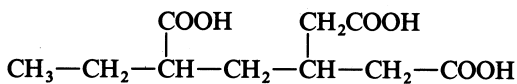


(1) Heptanoic acid

(2) 1-Hexanecarboxylic acid



(2) Cyclohexanecarboxylic acid



(3) 2-(Carboxymethyl)-1,4-hexanedicarboxylic acid

Removal of the OH from the  $\text{—COOH}$  group to form the acyl radical results in changing the ending -oic acid to -oyl or the ending -carboxylic acid to -carbonyl. Thus the radical  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CO—}$  is named either pentanoyl or butanecarbonyl. When the hydroxyl has not been removed from all carboxyl groups present in an acid, the remaining carboxyl groups are denoted by the prefix carboxy-. For example,  $\text{HOOCCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO—}$  is named 6-carboxyhexanoyl.

**TABLE 1.11** Names of Some Carboxylic Acids

| Systematic name               | Trivial name | Systematic name                                   | Trivial name   |
|-------------------------------|--------------|---------------------------------------------------|----------------|
| Methanoic                     | Formic       | <i>trans</i> -Methylbutenedioic                   | Mesaconic*     |
| Ethanoic                      | Acetic       |                                                   |                |
| Propanoic                     | Propionic    | 1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid | Camphoric      |
| Butanoic                      | Butyric      |                                                   |                |
| 2-Methylpropanoic             | Isobutyric*  |                                                   |                |
| Pentanoic                     | Valeric      | Benzenecarboxylic                                 | Benzoic        |
| 3-Methylbutanoic              | Isovaleric*  | 1,2-Benzenedicarboxylic                           | Phthalic       |
| 2,2-Dimethylpropanoic         | Pivalic*     | 1,3-Benzenedicarboxylic                           | Isophthalic    |
| Hexanoic                      | (Caproic)    | 1,4-Benzenedicarboxylic                           | Terephthalic   |
| Heptanoic                     | (Enanthic)   | Naphthalenecarboxylic                             | Naphthoic      |
| Octanoic                      | (Caprylic)   | Methylbenzenecarboxylic                           | Toluic         |
| Decanoic                      | (Capric)     | 2-Phenylpropanoic                                 | Hydratropic    |
| Dodecanoic                    | Lauric*      | 2-Phenylpropenoic                                 | Atropic        |
| Tetradecanoic                 | Myristic*    | <i>trans</i> -3-Phenylpropenoic                   | Cinnamic       |
| Hexadecanoic                  | Palmitic*    | Furancarboxylic                                   | Furoic         |
| Octadecanoic                  | Stearic*     | Thiophenecarboxylic                               | Thenoic        |
|                               |              | 3-Pyridinecarboxylic                              | Nicotinic      |
|                               |              | 4-Pyridinecarboxylic                              | Isonicotinic   |
| Ethanedioic                   | Oxalic       |                                                   |                |
| Propanedioic                  | Malonic      | Hydroxyethanoic                                   | Glycolic       |
| Butanedioic                   | Succinic     | 2-Hydroxypropanoic                                | Lactic         |
| Pentanedioic                  | Glutaric     | 2,3-Dihydroxypropanoic                            | Glyceric       |
| Hexanedioic                   | Adipic       | Hydroxypropanedioic                               | Tartronic      |
| Heptanedioic                  | Pimelic*     | Hydroxybutanedioic                                | Malic          |
| Octanedioic                   | Suberic*     | 2,3-Dihydroxybutanedioic                          | Tartaric       |
| Nonanedioic                   | Azelaic*     | 3-Hydroxy-2-phenylpropanoic                       | Tropic         |
| Decanedioic                   | Sebacic*     | 2-Hydroxy-2,2-diphenyl-ethanoic                   | Benzilic       |
| Propenoic                     | Acrylic      | 2-Hydroxybenzoic                                  | Salicylic      |
| Propynoic                     | Propiolic    | Methoxybenzoic                                    | Anisic         |
| 2-Methylpropenoic             | Methacrylic  | 4-Hydroxy-3-methoxybenzoic                        | Vanillic       |
| <i>trans</i> -2-Butenoic      | Crotonic     |                                                   |                |
| <i>cis</i> -2-Butenoic        | Isocrotonic  | 3,4-Dimethoxybenzoic                              | Veratric       |
| <i>cis</i> -9-Octadecenoic    | Oleic        | 3,4-Methylenedioxybenzoic                         | Piperonylic    |
| <i>trans</i> -9-Octadecenoic  | Elaidic      | 3,4-Dihydroxybenzoic                              | Protocatechuic |
| <i>cis</i> -Butenedioic       | Maleic       | 3,4,5-Trihydroxybenzoic                           | Gallic         |
| <i>trans</i> -Butenedioic     | Fumaric      |                                                   |                |
| <i>cis</i> -Methylbutenedioic | Citraconic*  |                                                   |                |

\* Systematic names should be used in derivatives formed by substitution on a carbon atom.

**Note:** The names in parentheses are abandoned but are listed for reference to older literature.

Many trivial names exist for acids; these are listed in Table 1.11. Generally, radicals are formed by replacing -ic acid by -oyl.\* When a trivial name is given to an acyclic monoacid or diacid, the numeral 1 is always given as locant to the carbon atom of a carboxyl group in the acid or to the carbon atom with a free valence in the radical RCO—.

\* Exceptions: formyl, acetyl, propionyl, butyryl, isobutyryl, valeryl, isovaleryl, oxalyl, malonyl, succinyl, glutaryl, furoyl, and thenoyl.

**1.1.3.13 Ethers ( $R^1-O-R^2$ ).** In substitutive nomenclature, one of the possible radicals,  $R-O-$ , is stated as the prefix to the parent compound that is senior from among  $R^1$  or  $R^2$ . Examples are methoxyethane for  $CH_3OCH_2CH_3$  and butoxyethanol for  $C_4H_9OCH_2CH_2OH$ .

When another principal group has precedence and oxygen is linking two identical parent compounds, the prefix oxy- may be used, as with 2,2'-oxydiethanol for  $HOCH_2CH_2OCH_2CH_2OH$ .

Compounds of the type  $RO-Y-OR$ , where the two parent compounds are identical and contain a group having priority over ethers for citation as suffix, are named as assemblies of identical units. For example,  $HOOC-CH_2-O-CH_2CH_2-O-CH_2-COOH$  is named 2,2'-(ethylene-dioxy)diacetic acid.

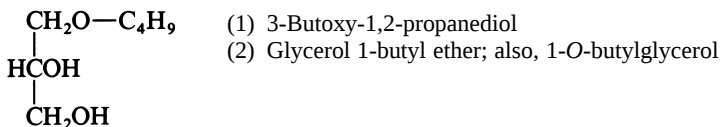
Linear polyethers derived from three or more molecules of aliphatic dihydroxy compounds, particularly when the chain length exceeds ten units, are most conveniently named by open-chain replacement nomenclature. For example,  $CH_3CH_2-O-CH_2CH_2-O-CH_2CH_3$  could be 3,6-dioxaoctane or (2-ethoxy)ethoxyethane.

An oxygen atom directly attached to two carbon atoms already forming part of a ring system or to two carbon atoms of a chain may be indicated by the prefix epoxy-. For example,  $CH_2-CH-O-CH_2Cl$  is named 1-chloro-2,3-epoxypropane.



Symmetrical linear polyethers may be named (1) in terms of the central oxygen atom when there is an odd number of ether oxygen atoms or (2) in terms of the central hydrocarbon group when there is an even number of ether oxygen atoms. For example,  $C_2H_5-O-C_4H_9-O-C_4H_9-O-C_2H_5$  is bis-(4-ethoxybutyl)ether, and 3,6-dioxaoctane (earlier example) could be named 1,2-bis-(ethoxy)ethane.

Partial ethers of polyhydroxy compounds may be named (1) by substitutive nomenclature or (2) by stating the name of the polyhydroxy compound followed by the name of the etherifying radical(s) followed by the word *ether*. For example,



Cyclic ethers are named either as heterocyclic compounds or by specialist rules of heterocyclic nomenclature. Radicofunctional names are formed by citing the names of the radicals  $R^1$  and  $R^2$  followed by the word *ether*. Thus methoxyethane becomes ethyl methyl ether and ethoxyethane becomes diethyl ether.

**1.1.3.14 Halogen Derivatives.** Using substitutive nomenclature, names are formed by adding prefixes listed in Table 1.8 to the name of the parent compound. The prefix perhalo- implies the replacement of all hydrogen atoms by the particular halogen atoms.

Cations of the type  $R^1R^2X^+$  are given names derived from the halonium ion,  $H_2X^+$ , by substitution, e.g., diethyliodonium chloride for  $(C_2H_5)_2I^+Cl^-$ .

Retained are these trivial names; bromoform ( $CHBr_3$ ), chloroform ( $CHCl_3$ ), fluoroform ( $CHF_3$ ), iodoform ( $CHI_3$ ), phosgene ( $COCl_2$ ), thiophosgene ( $CSCl_2$ ), and dichlorocarbene radical ( $\triangleright CCl_2$ ). Inorganic nomenclature leads to such names as carbonyl and thiocarbonyl halides ( $COX_2$  and  $CSX_2$ ) and carbon tetrahalides ( $CX_4$ ).

**1.1.3.15 Hydroxylamines and Oximes.** For  $RNH-OH$  compounds, prefix the name of the radical  $R$  to hydroxylamine. If another substituent has priority as principal group, attach the prefix

hydroxyamino- to the parent name. For example,  $\text{C}_6\text{H}_5\text{NHOH}$  would be named *N*-phenylhydroxylamine, but  $\text{HOC}_6\text{H}_4\text{NHOH}$  would be (hydroxyamino)phenol, with the point of attachment indicated by a locant preceding the parentheses.

Compounds of the type  $\text{R}^1\text{NH—OR}^2$  are named (1) as alkoxyamino derivatives of compound  $\text{R}^1\text{H}$ , (2) as *N,O*-substituted hydroxylamines, (3) as alkoxyamines (even if  $\text{R}^1$  is hydrogen), or (4) by the prefix aminooxy- when another substituent has priority for parent name. Examples of each type are

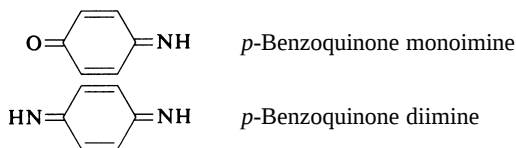
1. 2-(Methoxyamino)-8-naphthalenecarboxylic acid for  $\text{CH}_3\text{ONH—C}_{10}\text{H}_6\text{COOH}$
2. *O*-Phenylhydroxylamine for  $\text{H}_2\text{N—O—C}_6\text{H}_5$  or *N*-phenylhydroxylamine for  $\text{C}_6\text{H}_5\text{NH—OH}$
3. Phenoxyamine for  $\text{H}_2\text{N—O—C}_6\text{H}_5$  (not preferred to *O*-phenylhydroxylamine)
4. Ethyl (aminooxy)acetate for  $\text{H}_2\text{N—O—CH}_2\text{CO—OC}_2\text{H}_5$

Acyl derivatives,  $\text{RCO—NH—OH}$  and  $\text{H}_2\text{N—O—CO—R}$ , are named as *N*-hydroxy derivatives of amides and as *O*-acylhydroxylamines, respectively. The former may also be named as hydroxamic acids. Examples are *N*-hydroxyacetamide for  $\text{CH}_3\text{CO—NH—OH}$  and *O*-acetylhydroxylamine for  $\text{H}_2\text{N—O—CO—CH}_3$ . Further substituents are denoted by prefixes with *O*- and/or *N*-locants. For example,  $\text{C}_6\text{H}_5\text{NH—O—C}_2\text{H}_5$  would be *O*-ethyl-*N*-phenylhydroxylamine or *N*-ethoxylaniline.

For oximes, the word *oxime* is placed after the name of the aldehyde or ketone. If the carbonyl group is not the principal group, use the prefix hydroxyimino-. Compounds with the group  $\text{>N—OR}$  are named by a prefix alkoxyimino- as oxime *O*-ethers or as *O*-substituted oximes. Compounds with the group  $\text{>C=N(O)R}$  are named by adding *N*-oxide after the name of the alkylideneaminc compound. For amine oxides, add the word *oxide* after the name of the base, with locants. For example,  $\text{C}_5\text{H}_5\text{N—O}$  is named pyridine *N*-oxide or pyridine 1-oxide.

**1.1.3.16 Imines.** The group  $\text{>C=NH}$  is named either by the suffix -imine or by citing the name of the bivalent radical  $\text{R}^1\text{R}^2\text{C}<$  as a prefix to amine. For example,  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH=NH}$  could be named 1-butanimine or butylideneamine. When the nitrogen is substituted, as in  $\text{CH}_2=\text{N—CH}_2\text{CH}_3$ , the name is *N*-(methylidene)ethylamine.

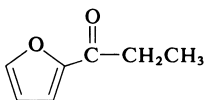
Quinones are exceptions. When one or more atoms of quinonoid oxygen have been replaced by  $\text{>NH}$  or  $\text{>NR}$ , they are named by using the name of the quinone followed by the word *imine* (and preceded by proper affixes). Substituents on the nitrogen atom are named as prefixes. Examples are



**1.1.3.17 Ketenes.** Derivatives of the compound ketene,  $\text{CH}_2=\text{C=O}$ , are named by substitutive nomenclature. For example,  $\text{C}_4\text{H}_9\text{CH=C=O}$  is butyl ketene. An acyl derivative, such as  $\text{CH}_3\text{CH}_2\text{—CO—CH}_2\text{CH=C=O}$ , may be named as a polyketone, 1-hexene-1,4-dione. Bisketene is used for two to avoid ambiguity with diketene (dimeric ketene).

**1.1.3.18 Ketones.** Acyclic ketones are named (1) by adding the suffix -one to the name of the hydrocarbon forming the principal chain or (2) by citing the names of the radicals  $\text{R}^1$  and  $\text{R}^2$  followed

by the word *ketone*. In addition to the preceding nomenclature, acyclic monoacyl derivatives of cyclic compounds may be named (3) by prefixing the name of the acyl group to the name of the cyclic compound. For example, the three possible names of

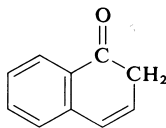


- (1) 1-(2-Furyl)-1-propanone
- (2) Ethyl 2-furyl ketone
- (3) 2-Propionylfuran

When the cyclic component is benzene or naphthalene, the -ic acid or -oic acid of the acid corresponding to the acyl group is changed to -ophenone or -onaphthone, respectively. For example,  $\text{C}_6\text{H}_5\text{—CO—CH}_2\text{CH}_2\text{CH}_3$  can be named either butyrophenone (or butanophenone) or phenyl propyl ketone.

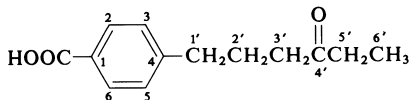
Radicalofunctional nomenclature can be used when a carbonyl group is attached directly to carbon atoms in two ring systems and no other substituent is present having priority for citation.

When the methylene group in polycarbocyclic and heterocyclic ketones is replaced by a keto group, the change may be denoted by attaching the suffix -one to the name of the ring system. However, when  $\geq\text{CH}$  in an unsaturated or aromatic system is replaced by a keto group, two alternative names become possible. First, the maximum number of noncumulative double bonds is added after introduction of the carbonyl group(s), and any hydrogen that remains to be added is denoted as indicated hydrogen with the carbonyl group having priority over the indicated hydrogen for lower-numbered locant. Second, the prefix oxo- is used, with the hydrogenation indicated by hydro prefixes; hydrogenation is considered to have occurred before the introduction of the carbonyl group. For example,

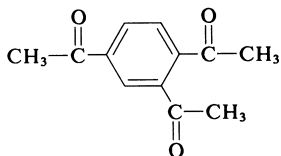


- (1) 1-(2H)-Naphthalenone
- (2) 1-Oxo-1,2-dihydronaphthalene

When another group having higher priority for citation as principal group is also present, the ketonic oxygen may be expressed by the prefix oxo-, or one can use the name of the carbonyl-containing radical, as, for example, acyl radicals and oxo-substituted radicals. Examples are



4-(4'-Oxohexyl)-1-benzoic acid

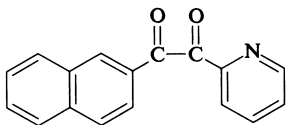


1,2,4-Triacetylbenzene

Diketones and tetraketones derived from aromatic compounds by conversion of two or four  $\geq\text{CH}$  groups into keto groups, with any necessary rearrangement of double bonds to a quinonoid structure, are named by adding the suffix -quinone and any necessary affixes.

Polyketones in which two or more contiguous carbonyl groups have rings attached at each end

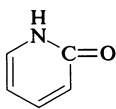
may be named (1) by the radicofunctional method or (2) by substitutive nomenclature. For example,



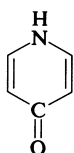
- (1) 2-Naphthyl 2-pyridyl diketone  
(2) 1-(2-Naphthyl)-2-(2-pyridyl)ethanedione

Some trivial names are retained: acetone (2-propanone), biacetyl (2,3-butanedione), propiophenone ( $\text{C}_6\text{H}_5-\text{CO}-\text{CH}_2\text{CH}_3$ ), chalcone ( $\text{C}_6\text{H}_5-\text{CH}=\text{CH}-\text{CO}-\text{C}_6\text{H}_5$ ), and deoxybenzoin ( $\text{C}_6\text{H}_5-\text{CH}_2-\text{CO}-\text{C}_6\text{H}_5$ ).

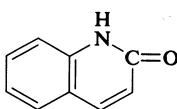
These contracted names of heterocyclic nitrogen compounds are retained as alternatives for systematic names, sometimes with indicated hydrogen. In addition, names of oxo derivatives of fully saturated nitrogen heterocycles that systematically end in -idinone are often contracted to end in -idone when no ambiguity might result. For example,



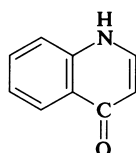
2-Pyridone  
2(1H)-Pyridone



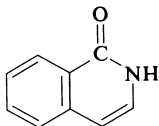
4-Pyridone  
4(1H)-Pyridone



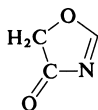
2-Quinolone  
2(1H)-Quinolone



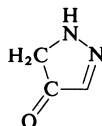
4-Quinolone  
4(1H)-Quinolone



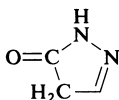
1-Isoquinolone  
1(2H)-Isoquinolone



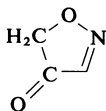
4-Oxazolone  
4(5H)-Oxazolone



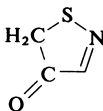
4-Pyrazolone  
4(5H)-Pyrazolone



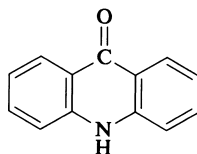
5-Pyrazolone  
5(4H)-Pyrazolone



4-Isioxazoline  
4(5H)-Isioxazoline



4-Thiazolone  
4(5H)-Thiazolone



9-Acrindone  
9(10H)-Acrindone

**1.1.3.19 Lactones, Lactides, Lactams, and Lactims.** When the hydroxy acid from which water may be considered to have been eliminated has a trivial name, the lactone is designated by substituting -olactone for -ic acid. Locants for a carbonyl group are numbered as low as possible, even before that of a hydroxyl group.

Lactones formed from aliphatic acids are named by adding -olide to the name of the nonhydroxylated hydrocarbon with the same number of carbon atoms. The suffix -olide signifies the change of  $\text{>CH}\cdots\text{CH}_3$  into  $\text{>C}\cdots\text{C=O}$ .



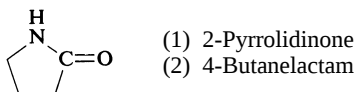
Structures in which one or more (but not all) rings of an aggregate are lactone rings are named by placing -carbolactone (denoting the  $\text{—O—CO—}$  bridge) after the names of the structures that



remain when each bridge is replaced by two hydrogen atoms. The locant for  $\text{—CO—}$  is cited before that for the ester oxygen atom. An additional carbon atom is incorporated into this structure as compared to the -olide.

These trivial names are permitted:  $\gamma$ -butyrolactone,  $\gamma$ -valerolactone, and  $\delta$ -valerolactone. Names based on heterocycles may be used for all lactones. Thus,  $\gamma$ -butyrolactone is also tetrahydro-2-furanone or dihydro-2(3H)-furanone.

*Lactides*, intermolecular cyclic esters, are named as heterocycles. *Lactams* and *lactims*, containing a  $\text{—CO—NH—}$  and  $\text{—C(OH)=N—}$  group, respectively, are named as heterocycles, but they may also be named with -lactam or -lactim in place of -olide. For example,



**1.1.3.20 Nitriles and Related Compounds.** For acids whose systematic names end in -carboxylic acid, nitriles are named by adding the suffix -carbonitrile when the  $\text{—CN}$  group replaces the  $\text{—COOH}$  group. The carbon atom of the  $\text{—CN}$  group is excluded from the numbering of a chain to which it is attached. However, when the triple-bonded nitrogen atom is considered to replace three hydrogen atoms at the end of the main chain of an acyclic hydrocarbon, the suffix -nitrile is added to the name of the hydrocarbon. Numbering begins with the carbon attached to the nitrogen. For example,  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CN}$  is named (1) pentanecarbonitrile or (2) hexanenitrile.

Trivial acid names are formed by changing the endings -oic acid or -ic acid to -onitrile. For example,  $\text{CH}_3\text{CN}$  is acetonitrile. When the  $\text{—CN}$  group is not the highest priority group, the  $\text{—CN}$  group is denoted by the prefix cyano-.

In order of decreasing priority for citation of a functional class name, and the prefix for substitutive nomenclature, are the following related compounds:

| Functional group | Prefix            | Radicofunctional ending |
|------------------|-------------------|-------------------------|
| $\text{—NC}$     | Isocyano-         | Isocyanide              |
| $\text{—OCN}$    | Cyanato-          | Cyanate                 |
| $\text{—NCO}$    | Isocyanato-       | Isocyanate              |
| $\text{—ONC}$    | —                 | Fulminate               |
| $\text{—SCN}$    | Thiocyanato-      | Thiocyanate             |
| $\text{—NCS}$    | Isothiocyanato-   | Isothiocyanate          |
| $\text{—SeCN}$   | Selenocyanato-    | Selenocyanate           |
| $\text{—NCSe}$   | Isoselenocyanato- | Isoselenocyanate        |

**1.1.3.21 Peroxides.** Compounds of the type  $\text{R—O—OH}$  are named (1) by placing the name of the radical R before the word *hydroperoxide* or (2) by use of the prefix *hydroperoxy-* when another parent name has higher priority. For example,  $\text{C}_2\text{H}_5\text{OOH}$  is ethyl hydroperoxide.

Compounds of the type  $\text{R}^1\text{O—OR}^2$  are named (1) by placing the names of the radicals in alphabetical order before the word *peroxide* when the group  $\text{—O—O—}$  links two chains, two rings, or a ring and a chain, (2) by use of the affix *dioxy* to denote the bivalent group  $\text{—O—O—}$  for naming assemblies of identical units or to form part of a prefix, or (3) by use of the prefix *epidioxy-* when the peroxide group forms a bridge between two carbon atoms, a ring, or a ring system.

Examples are methyl propyl peroxide for  $\text{CH}_3\text{—O—O—C}_3\text{H}_7$  and 2,2'-dioxydiacetic acid for  $\text{HOOC—CH}_2\text{—O—O—CH}_2\text{—COOH}$ .

**1.1.3.22 Phosphorus Compounds.** Acyclic phosphorus compounds containing only one phosphorus atom, as well as compounds in which only a single phosphorus atom is in each of several functional groups, are named as derivatives of the parent structures listed in Table 1.12. Often these

**TABLE 1.12** Parent Structures of Phosphorus-Containing Compounds

| Formula                                                                                                                                                                                                                              | Parent name                                                                                                                                               | Substitutive prefix                                                                                                                                                                                                                                   | Radicofunctional ending                                                |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------|
| $\text{H}_3\text{P}$<br>$\text{H}_5\text{P}$                                                                                                                                                                                         | Phosphine<br>Phosphorane                                                                                                                                  | $\text{H}_2\text{P—}$ Phosphino-<br>$\text{H}_4\text{P—}$ Phosphoranyl-<br>$\text{H}_3\text{P} \leq$ Phosphoroanediyl-<br>$\text{H}_2\text{P} \leq$ Phosphoranetriyl-                                                                                 | Phosphide                                                              |
| $\text{H}_3\text{PO}$<br>$\text{H}_3\text{PS}$<br>$\text{H}_3\text{PNH}$<br>$\text{P}(\text{OH})_3$<br>$\text{HP}(\text{OH})_2$<br>$\text{H}_2\text{POH}$<br>$\text{P}(\text{O})(\text{OH})_3$<br>$\text{HP}(\text{O})(\text{OH})_2$ | Phosphine oxide<br>Phosphine sulfide<br>Phosphine imide<br>Phosphorous acid<br>Phosphonous acid<br>Phosphinous acid<br>Phosphoric acid<br>Phosphonic acid | $\text{P}(\text{O}) \leq$ Phosphoryl-<br>$\text{HP}(\text{O}) \leq$ Phosphonoyl-<br>$\text{—P}(\text{O})\text{OH}_2$ Phosphono-<br>$\text{H}_2\text{P}(\text{O})\text{—}$ Phosphinoyl-<br>$\text{>P}(\text{O})\text{OH}$ Phosphinoco-<br>Phosphinato- | Phosphite<br>Phosphonite<br>Phosphinite<br>Phosphate(V)<br>Phosphonate |
| $\text{H}_2\text{P}(\text{O})\text{OH}$                                                                                                                                                                                              | Phosphinic acid                                                                                                                                           |                                                                                                                                                                                                                                                       | Phosphinate                                                            |

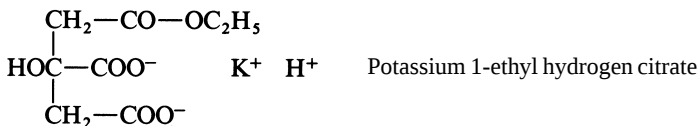
are purely hypothetical parent structures. When hydrogen attached to phosphorus is replaced by a hydrocarbon group, the derivative is named by substitution nomenclature. When hydrogen of an  $\text{—OH}$  group is replaced, the derivative is named by radicofunctional nomenclature. For example,  $\text{C}_2\text{H}_5\text{PH}_2$  is ethylphosphine;  $(\text{C}_2\text{H}_5)_2\text{PH}$ , diethylphosphine;  $\text{CH}_3\text{P}(\text{OH})_2$ , dihydroxy-methyl-phosphine or methylphosphonous acid;  $\text{C}_2\text{H}_5\text{—PO}(\text{Cl})(\text{OH})$ , ethylchlorophosphonic acid or ethylphosphonochloridic acid or hydrogen chlorodioxoethylphosphate(V);  $\text{CH}_3\text{CH}(\text{PH}_2)\text{COOH}$ , 2-phosphinopropionic acid;  $\text{HP}(\text{CH}_2\text{COOH})_2$ , phosphinediylacetic acid;  $(\text{CH}_3)\text{HP}(\text{O})\text{OH}$ , methylphosphinic acid or hydrogen hydridomethyl dioxophosphate(V);  $(\text{CH}_3\text{O})_3\text{PO}$ , trimethyl phosphate; and  $(\text{CH}_3\text{O})_3\text{P}$ , trimethyl phosphite.

**1.1.3.23 Salts and Esters of Acids.** Neutral salts of acids are named by citing the cation(s) and then the anion, whose ending is changed from -oic to -oate or from -ic to -ate. When different acidic residues are present in one structure, prefixes are formed by changing the anion ending -ate to -ato- or -ide to -ido-. The prefix carboxylato- denotes the ionic group  $\text{—COO}^-$ . The phrase (metal) salt of (the acid) is permissible when the carboxyl groups are not all named as affixes.

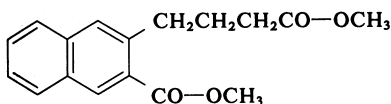
Acid salts include the word *hydrogen* (with affixes, if appropriate) inserted between the name of the cation and the name of the anion (or word *salt*).

Esters are named similarly, with the name of the alkyl or aryl radical replacing the name of the

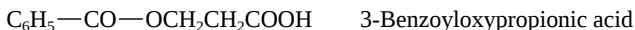
cation. Acid esters of acids and their salts are named as neutral esters, but the components are cited in the order: cation, alkyl or aryl radical, hydrogen, and anion. Locants are added if necessary. For example,



Ester groups in  $\text{R}^1\text{—CO—OR}^2$  compounds are named (1) by the prefix alkoxycarbonyl- or aryloxy carbonyl- for  $\text{—CO—OR}^2$  when the radical  $\text{R}^1$  contains a substituent with priority for citation as principal group or (2) by the prefix acyloxy- for  $\text{R}^1\text{—CO—O—}$  when the radical  $\text{R}^2$  contains a substituent with priority for citation as principal group. Examples are



Methyl 3-methoxycarbonyl-2-naphthalenebutyrate



The trivial name *acetox*y is retained for the  $\text{CH}_3\text{—CO—O—}$  group. Compounds of the type  $\text{R}^2\text{C(OR}^3)_3$  are named as  $\text{R}^2$  esters of the hypothetical ortho acids. For example,  $\text{CH}_3\text{C(OCH}_3)_3$  is trimethyl orthoacetate.

**1.1.3.24 Silicon Compounds.**  $\text{SiH}_4$  is called silane; its acyclic homologs are called disilane, trisilane, and so on, according to the number of silicon atoms present. The chain is numbered from one end to the other so as to give the lowest-numbered locant in radicals to the free valence or to substituents on a chain. The abbreviated form silyl is used for the radical  $\text{SiH}_3\text{—}$ . Numbering and citation of side chains proceed according to the principles set forth for hydrocarbon chains. Cyclic nonaromatic structures are designated by the prefix *cyclo-*.

When a chain or ring system is composed entirely of alternating silicon and oxygen atoms, the parent name *siloxane* is used with a multiplying affix to denote the number of silicon atoms present. The parent name *silazane* implies alternating silicon and nitrogen atoms; multiplying affixes denote the number of silicon atoms present.

The prefix *sila-* designates replacement of carbon by silicon in replacement nomenclature. Prefix names for radicals are formed analogously to those for the corresponding carbon-containing compounds. Thus silyl is used for  $\text{SiH}_3\text{—}$ , silylene for  $\text{—SiH}_2\text{—}$ , silylidyne for  $\text{—SiH<}$ , as well as trily, tetrayl, and so on for free valences(s) on ring structures.

#### 1.1.3.25 Sulfur Compounds

**Bivalent Sulfur.** The prefix *thio*, placed before an affix that denotes the oxygen-containing group or an oxygen atom, implies the replacement of that oxygen by sulfur. Thus the suffix *-thiol* denotes  $\text{—SH}$ , *-thione* denotes  $\text{—(C)=S}$  and implies the presence of an  $\text{=S}$  at a nonterminal carbon atom, *-thioic acid* denotes  $[(\text{C})=\text{S}]\text{OH} \rightleftharpoons [(\text{C})=\text{O}]\text{SH}$  (that is, the *O*-substituted acid and the *S*-substi-

tuted acid, respectively), -dithioc acid denotes  $[\text{—C(S)}]\text{SH}$ , and -thial denotes  $\text{—(C)HS}$  (or -carbothialdehyde denotes  $\text{—CHS}$ ). When -carboxylic acid has been used for acids, the sulfur analog is named -carbothioic acid or -carbodithioic acid.

Prefixes for the groups  $\text{HS—}$  and  $\text{RS—}$  are mercapto- and alkylthio-, respectively; this latter name may require parentheses for distinction from the use of thio- for replacement of oxygen in a trivially named acid. Examples of this problem are  $4\text{-C}_2\text{H}_5\text{—C}_6\text{H}_4\text{—CSOH}$  named *p*-ethyl(thio)benzoic acid and  $4\text{-C}_2\text{H}_5\text{—S—C}_6\text{H}_4\text{—COOH}$  named *p*-(ethylthio)benzoic acid. When  $\text{—SH}$  is not the principal group, the prefix mercapto- is placed before the name of the parent compound to denote an unsubstituted  $\text{—SH}$  group.

The prefix thioxo- is used for naming  $\text{=S}$  in a thioketone. Sulfur analogs of acetals are named as alkylthio- or arylthio-. For example,  $\text{CH}_3\text{CH}(\text{SCH}_3)\text{OCH}_3$  is 1-methoxy-1-(methylthio)ethane. Prefix forms for -carbothioic acids are hydroxy(thiocarbonyl)- when referring to the *O*-substituted acid and mercapto(carbonyl)- for the *S*-substituted acid.

Salts are formed as with oxygen-containing compounds. For example,  $\text{C}_2\text{H}_5\text{—S—Na}$  is named either sodium ethanethiolate or sodium ethyl sulfide. If mercapto- has been used as a prefix, the salt is named by use of the prefix sulfido- for  $\text{—S}^-$ .

Compounds of the type  $\text{R}^1\text{—S—R}^2$  are named alkylthio- (or arylthio-) as a prefix to the name of  $\text{R}^1$  or  $\text{R}^2$ , whichever is the senior.

**Sulfonium Compounds.** Sulfonium compounds of the type  $\text{R}^1\text{R}^2\text{R}^3\text{S}^+\text{X}^-$  are named by citing in alphabetical order the radical names followed by -sulfonium and the name of the anion. For heterocyclic compounds, -ium is added to the name of the ring system. Replacement of  $>\text{CH}$  by sulfonium sulfur is denoted by the prefix thionia-, and the name of the anion is added at the end.

**Organosulfur Halides.** When sulfur is directly linked only to an organic radical and to a halogen atom, the radical name is attached to the word *sulfur* and the name(s) and number of the halide(s) are stated as a separate word. Alternatively, the name can be formed from  $\text{R—SOH}$ , a sulfenic acid whose radical prefix is sulfenyl-. For example,  $\text{CH}_3\text{CH}_2\text{—S—Br}$  would be named either ethylsulfur monobromide or ethanesulfenyl bromide. When another principal group is present, a composite prefix is formed from the number and substitutive name(s) of the halogen atoms in front of the syllable thio. For example,  $\text{BrS—COOH}$  is (bromothio)formic acid.

**Sulfoxides.** Sulfoxides,  $\text{R}^1\text{—SO—R}^2$ , are named by placing the names of the radicals in alphabetical order before the word *sulfoxide*. Alternatively, the less senior radical is named followed by sulfinyl- and concluded by the name of the senior group. For example,  $\text{CH}_3\text{CH}_2\text{—SO—CH}_2\text{CH}_2\text{CH}_3$  is named either ethyl propyl sulfoxide or 1-(ethylsulfinyl)propane.

When an  $>\text{SO}$  group is incorporated in a ring, the compound is named an oxide.

**Sulfones.** Sulfones,  $\text{R}^1\text{—SO}_2\text{—R}^2$ , are named in an analogous manner to sulfoxides, using the word *sulfone* in place of *sulfoxide*. In prefixes, the less senior radical is followed by -sulfonyl-. When the  $>\text{SO}_2$  group is incorporated in a ring, the compound is named as a dioxide.

**Sulfur Acids.** Organic oxy acids of sulfur, that is,  $\text{—SO}_3\text{H}$ ,  $\text{—SO}_2\text{H}$ , and  $\text{—SOH}$ , are named sulfonic acid, sulfinic acid, and sulfenic acid, respectively. In subordinate use, the respective prefixes are sulfo-, sulfinio, and sulfeno-. The grouping  $\text{—SO}_2\text{—O—SO}_2\text{—}$  or  $\text{—SO—O—SO—}$  is named sulfonic or sulfinic anhydride, respectively.

Inorganic nomenclature is employed in naming sulfur acids and their derivatives in which sulfur is linked only through oxygen to the organic radical. For example,  $(\text{C}_2\text{H}_5\text{O})_2\text{SO}_2$  is diethyl sulfate and  $\text{C}_2\text{H}_5\text{O—SO}_2\text{—OH}$  is ethyl hydrogen sulfate. Prefixes *O*- and *S*- are used where necessary to denote attachment to oxygen and to sulfur, respectively, in sulfur replacement compounds. For example,  $\text{CH}_3\text{—S—SO}_2\text{—ONa}$  is sodium *S*-methyl thiosulfate.

When sulfur is linked only through nitrogen, or through nitrogen and oxygen, to the organic radical, naming is as follows: (1) *N*-substituted amides are designated as *N*-substituted derivatives of the sulfur amides and (2) compounds of the type  $\text{R—NH—SO}_3\text{H}$  may be named as *N*-substituted

sulfamic acids or by the prefix sulfoamino- to denote the group  $\text{HO}_3\text{S}-\text{NH}-$ . The groups  $-\text{N}=\text{SO}$  and  $-\text{N}=\text{SO}_2$  are named sulfinylamines and sulfonylamines, respectively.

**Sultones and Sultams.** Compounds containing the group  $-\text{SO}_2-\text{O}-$  as part of the ring are called -sultone. The  $-\text{SO}_2-$  group has priority over the  $-\text{O}-$  group for lowest-numbered locant.

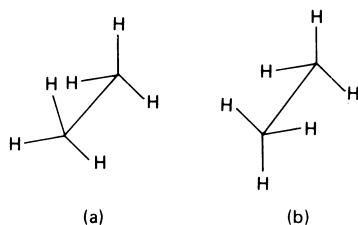
Similarly, the  $-\text{SO}_2-\text{N}=\text{}$  group as part of a ring is named by adding -sultam to the name of the hydrocarbon with the same number of carbon atoms. The  $-\text{SO}_2-$  has priority over  $-\text{N}=\text{}$  for lowest-numbered locant.

### 1.1.4 Stereochemistry

Concepts in stereochemistry, that is, chemistry in three-dimensional space, are in the process of rapid expansion. This section will deal with only the main principles. The compounds discussed will be those that have identical molecular formulas but differ in the arrangement of their atoms in space. *Stereoisomers* is the name applied to these compounds.

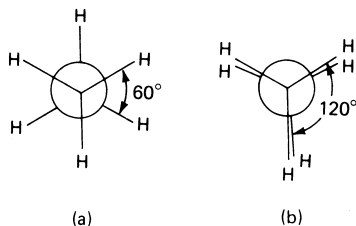
Stereoisomers can be grouped into three categories: (1) Conformational isomers differ from each other only in the way their atoms are oriented in space, but can be converted into one another by rotation about sigma bonds. (2) Geometric isomers are compounds in which rotation about a double bond is restricted. (3) Configurational isomers differ from one another only in configuration about a chiral center, axis, or plane. In subsequent structural representations, a broken line denotes a bond projecting behind the plane of the paper and a wedge denotes a bond projecting in front of the plane of the paper. A line of normal thickness denotes a bond lying essentially in the plane of the paper.

**1.1.4.1 Conformational Isomers.** A molecule in a conformation into which its atoms return spontaneously after small displacements is termed a *conformer*. Different arrangements of atoms that can be converted into one another by rotation about single bonds are called *conformational isomers* (see Fig. 1.1). A pair of conformational isomers can be but do not have to be mirror images of each other. When they are not mirror images, they are called *diastereomers*.



**FIGURE 1.1** Conformations of ethane.  
(a) Eclipsed; (b) staggered.

**Acyclic Compounds.** Different conformations of acyclic compounds are best viewed by construction of ball-and-stick molecules or by use of Newman projections (see Fig. 1.2). Both types of representations are shown for ethane. Atoms or groups that are attached at opposite ends of a single bond should be viewed along the bond axis. If two atoms or groups attached at opposite ends of the bond appear one directly behind the other, these atoms or groups are described as eclipsed. That portion of the molecule is described as being in the eclipsed conformation. If not eclipsed, the atoms

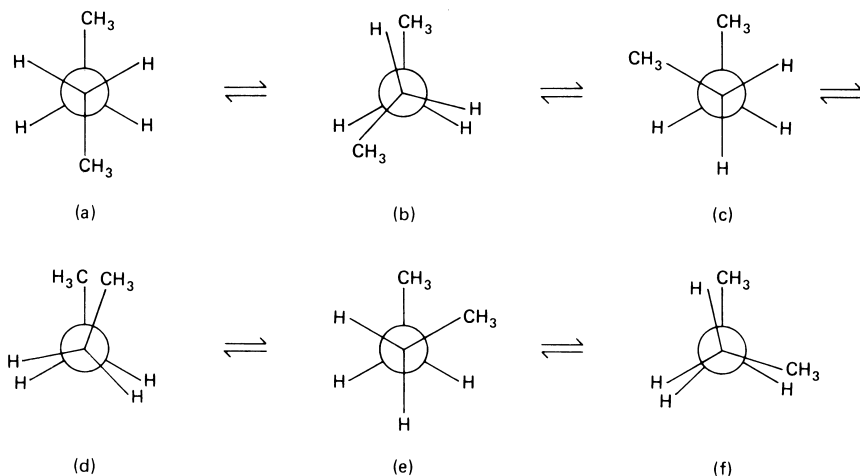


**FIGURE 1.2** Newman projections for ethane. (a) Staggered; (b) eclipsed.

or groups and the conformation may be described as staggered. Newman projections show these conformations clearly.

Certain physical properties show that rotation about the single bond is not quite free. For ethane there is an energy barrier of about  $3 \text{ kcal} \cdot \text{mol}^{-1}$  ( $12 \text{ kJ} \cdot \text{mol}^{-1}$ ). The potential energy of the molecule is at a minimum for the staggered conformation, increases with rotation, and reaches a maximum at the eclipsed conformation. The energy required to rotate the atoms or groups about the carbon-carbon bond is called *torsional energy*. Torsional strain is the cause of the relative instability of the eclipsed conformation or any intermediate skew conformations.

In butane, with a methyl group replacing one hydrogen on each carbon of ethane, there are several different staggered conformations (see Fig. 1.3). There is the *anti*-conformation in which the methyl groups are as far apart as they can be (dihedral angle of  $180^\circ$ ). There are two *gauche* conformations in which the methyl groups are only  $60^\circ$  apart; these are two nonsuperimposable mirror images of each other. The *anti*-conformation is more stable than the *gauche* by about  $0.9 \text{ kcal} \cdot \text{mol}^{-1}$  ( $4 \text{ kJ} \cdot \text{mol}^{-1}$ ). Both are free of torsional strain. However, in a *gauche* conformation the methyl groups are closer together than the sum of their van der Waals' radii. Under these conditions van der Waals' forces are repulsive and raise the energy of conformation. This strain can affect not only the relative stabilities of various staggered conformations but also the heights of the energy barriers



**FIGURE 1.3** Conformations of butane. (a) *Anti*-staggered; (b) eclipsed; (c) *gauche*-staggered; (d) eclipsed; (e) *gauche*-staggered; (f) eclipsed. (Eclipsed conformations are slightly staggered for convenience in drawing; actually they are superimposed.)

between them. The energy maximum (estimated at  $4.8$  to  $6.1 \text{ kcal} \cdot \text{mol}^{-1}$  or  $20$  to  $25 \text{ kJ} \cdot \text{mol}^{-1}$ ) is reached when two methyl groups swing past each other (the eclipsed conformation) rather than past hydrogen atoms.

**Cyclic Compounds.** Although cyclic aliphatic compounds are often drawn as if they were planar geometric figures (a triangle for cyclopropane, a square for cyclobutane, and so on), their structures are not that simple. Cyclopropane does possess the maximum angle strain if one considers the difference between a tetrahedral angle ( $109.5^\circ$ ) and the  $60^\circ$  angle of the cyclopropane structure. Nevertheless the cyclopropane structure is thermally quite stable. The highest electron density of the carbon-carbon bonds does not lie along the lines connecting the carbon atoms. Bonding electrons lie principally outside the triangular internuclear lines and result in what is known as *bent bonds* (see Fig. 1.4).

Cyclobutane has less angle strain than cyclopropane (only  $19.5^\circ$ ). It is also believed to have some bent-bond character associated with the carbon-carbon bonds. The molecule exists in a nonplanar conformation in order to minimize hydrogen-hydrogen eclipsing strain.

Cyclopentane is nonplanar, with a structure that resembles an envelope (see Fig. 1.5). Four of the carbon atoms are in one plane, and the fifth is out of that plane. The molecule is in continual motion so that the out-of-plane carbon moves rapidly around the ring.

The 12 hydrogen atoms of cyclohexane do not occupy equivalent positions. In the chair conformation six hydrogen atoms are perpendicular to the average plane of the molecule and six are directed outward from the ring, slightly above or below the molecular plane (see Fig. 1.6). Bonds which are perpendicular to the molecular plane are known as *axial bonds*, and those which extend outward

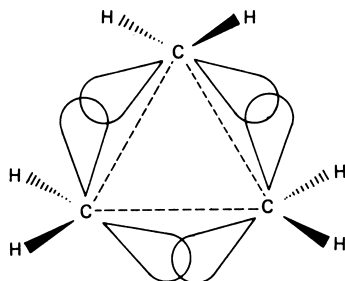


FIGURE 1.4 The bent bonds ("tear drops") of cyclopropane.

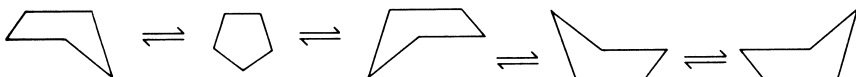


FIGURE 1.5 The conformations of cyclopentane.

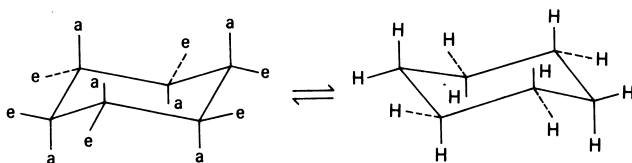
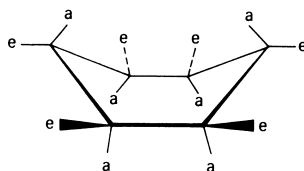


FIGURE 1.6 The two chair conformations of cyclohexane; *a* = axial hydrogen atom and *e* = equatorial hydrogen atom.

from the ring are known as *equatorial bonds*. The three axial bonds directed upward originate from alternate carbon atoms and are parallel with each other; a similar situation exists for the three axial bonds directed downward. Each equatorial bond is drawn so as to be parallel with the ring carbon-carbon bond once removed from the point of attachment to that equatorial bond. At room temperature, cyclohexane is interconverting rapidly between two chair conformations. As one chair form converts to the other, all the equatorial hydrogen atoms become axial and all the axial hydrogens become equatorial. The interconversion is so rapid that all hydrogen atoms on cyclohexane can be considered equivalent. Interconversion is believed to take place by movement of one side of the chair structure to produce the twist boat, and then movement of the other side of the twist boat to give the other chair form. The chair conformation is the most favored structure for cyclohexane. No angle strain is encountered since all bond angles remain tetrahedral. Torsional strain is minimal because all groups are staggered.

In the boat conformation of cyclohexane (Fig. 1.7) eclipsing torsional strain is significant, although no angle strain is encountered. Nonbonded interaction between the two hydrogen atoms across the ring from each other (the “flagpole” hydrogens) is unfavorable. The boat conformation is about  $6.5 \text{ kcal} \cdot \text{mol}^{-1}$  ( $27 \text{ kJ} \cdot \text{mol}^{-1}$ ) higher in energy than the chair form at  $25^\circ\text{C}$ .



**FIGURE 1.7** The boat conformation of cyclohexane. *a* = axial hydrogen atom and *e* = equatorial hydrogen atom.



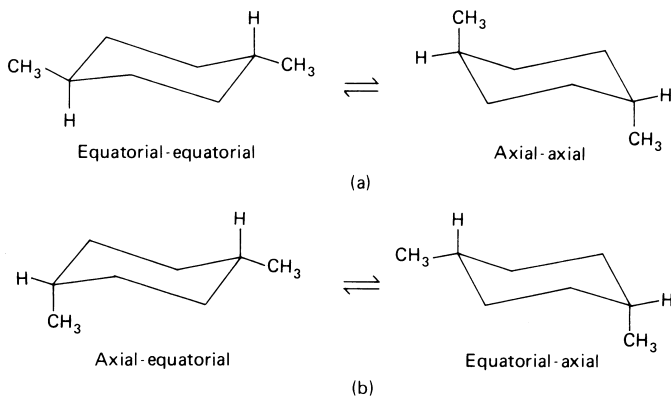
**FIGURE 1.8** Twist-boat conformation of cyclohexane.

A modified boat conformation of cyclohexane, known as the twist boat (Fig. 1.8), or skew boat, has been suggested to minimize torsional and nonbonded interactions. This particular conformation is estimated to be about  $1.5 \text{ kcal} \cdot \text{mol}^{-1}$  ( $6 \text{ kJ} \cdot \text{mol}^{-1}$ ) lower in energy than the boat form at room temperature.

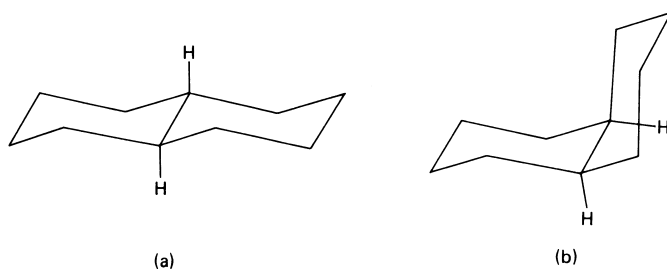
The medium-size rings (7 to 12 ring atoms) are relatively free of angle strain and can easily take a variety of spatial arrangements. They are not large enough to avoid all nonbonded interactions between atoms.

Disubstituted cyclohexanes can exist as *cis-trans* isomers as well as axial-equatorial conformers. Two isomers are predicted for 1,4-dimethylcyclohexane (see Fig. 1.9). For the *trans* isomer the diequatorial conformer is the energetically favorable form. Only one *cis* isomer is observed, since the two conformers of the *cis* compound are identical. Interconversion takes place between the conformational (equatorial-axial) isomers but not configurational (*cis-trans*) isomers.





**FIGURE 1.9** Two isomers of 1,4-dimethylcyclohexane. (a) *Trans* isomer; (b) *cis* isomer.



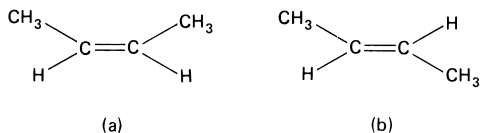
**FIGURE 1.10** Two isomers of decahydronaphthalene, or bicyclo[4.4.0]decane. (a) *Trans* isomer; (b) *cis* isomer.

The bicyclic compound decahydronaphthalene, or bicyclo[4.4.0]decane, has two fused six-membered rings. It exists in *cis* and *trans* forms (see Fig. 1.10), as determined by the configurations at the bridgehead carbon atoms. Both *cis*- and *trans*-decahydronaphthalene can be constructed with two chair conformations.

**1.1.4.2 Geometrical Isomerism.** Rotation about a carbon-carbon double bond is restricted because of interaction between the *p* orbitals which make up the pi bond. Isomerism due to such restricted rotation about a bond is known as *geometric isomerism*. Parallel overlap of the *p* orbitals of each carbon atom of the double bond forms the molecular orbital of the pi bond. The relatively large barrier to rotation about the pi bond is estimated to be nearly  $63 \text{ kcal} \cdot \text{mol}^{-1}$  ( $263 \text{ kJ} \cdot \text{mol}^{-1}$ ).

When two different substituents are attached to each carbon atom of the double bond, *cis-trans* isomers can exist. In the case of *cis*-2-butene (Fig. 1.11a), both methyl groups are on the same side of the double bond. The other isomer has the methyl groups on opposite sides and is designated as *trans*-2-butene (Fig. 1.11b). Their physical properties are quite different. Geometric isomerism can also exist in ring systems; examples were cited in the previous discussion on conformational isomers.

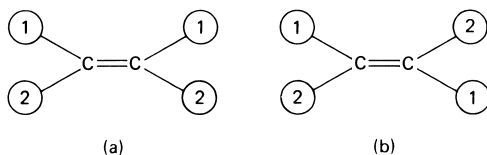
For compounds containing only double-bonded atoms, the reference plane contains the double-bonded atoms and is perpendicular to the plane containing these atoms and those directly attached to them. It is customary to draw the formulas so that the reference plane is perpendicular to that of



**FIGURE 1.11** Two isomers of 2-butene. (a) *Cis* isomer, bp 3.8°C, mp −138.9°C, dipole moment 0.33 D; (b) *trans* isomer, bp 0.88°C, mp −105.6°C, dipole moment 0 D.

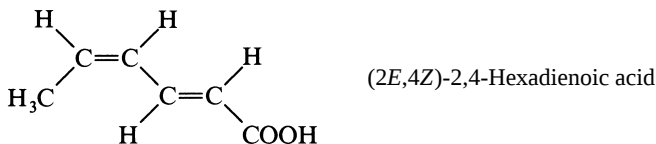
the paper. For cyclic compounds the reference plane is that in which the ring skeleton lies or to which it approximates. Cyclic structures are commonly drawn with the ring atoms in the plane of the paper.

**1.1.4.3 Sequence Rules for Geometric Isomers and Chiral Compounds.** Although *cis* and *trans* designations have been used for many years, this approach becomes useless in complex systems. To eliminate confusion when each carbon of a double bond or a chiral center is connected to different groups, the Cahn, Ingold, and Prelog system for designating configuration about a double bond or a chiral center has been adopted by IUPAC. Groups on each carbon atom of the double bond are assigned a first (1) or second (2) priority. Priority is then compared at one carbon relative to the other. When both first priority groups are on the *same side* of the double bond, the configuration is designated as *Z* (from the German *zusammen*, “together”), which was formerly *cis*. If the first priority groups are on *opposite sides* of the double bond, the designation is *E* (from the German *entgegen*, “in opposition to”), which was formerly *trans*. (See Fig. 1.12.)



**FIGURE 1.12** Configurations designated by priority groups. (a) *Z* (*cis*); (b) *E* (*trans*).

When a molecule contains more than one double bond, each *E* or *Z* prefix has associated with it the lower-numbered locant of the double bond concerned. Thus (see also the rules that follow)



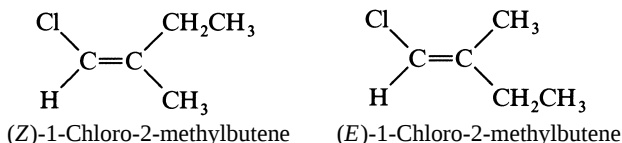
When the sequence rules permit alternatives, preference for lower-numbered locants and for inclusion in the principal chain is allotted as follows in the order stated: *Z* over *E* groups and *cis* over *trans* cyclic groups. If a choice is still not attained, then the lower-numbered locant for such a preferred

group at the first point of difference is the determining factor. For example,



**Rule 1.** Priority is assigned to atoms on the basis of atomic number. Higher priority is assigned to atoms of higher atomic number. If two atoms are isotopes of the same element, the atom of higher mass number has the higher priority. For example, in 2-butene, the carbon atom of each methyl group receives first priority over the hydrogen atom connected to the same carbon atom. Around the asymmetric carbon atom in chloriodomethanesulfonic acid, the priority sequence is I, Cl, S, H. In 1-bromo-1-deuteroethane, the priority sequence is Cl, C, D, H.

**Rule 2.** When atoms attached directly to a double-bonded carbon have the same priority, the second atoms are considered and so on, if necessary, working outward once again from the double bond or chiral center. For example, in 1-chloro-2-methylbutene, in  $\text{CH}_3$  the second atoms are H, H, H and in  $\text{CH}_2\text{CH}_3$  they are C, H, H. Since carbon has a higher atomic number than hydrogen, the ethyl group has the next highest priority after the chlorine atom.



**Rule 3.** When groups under consideration have double or triple bonds, the multiple-bonded atom is replaced conceptually by two or three single bonds to that same kind of atom.

Thus,  $=\text{A}$  is considered to be equivalent to two A's, or  $\begin{smallmatrix} \text{A} \\ < \\ \text{A} \end{smallmatrix}$  and  $\equiv\text{A}$  equals  $\begin{smallmatrix} \text{A} & & \text{A} \\ < & & < \\ \text{A} & & \text{A} \end{smallmatrix}$ . However, a real  $\begin{smallmatrix} \text{A} \\ < \\ \text{A} \end{smallmatrix}$  has priority over  $=\text{A}$ ; likewise a real  $\begin{smallmatrix} \text{A} & & \text{A} \\ < & & < \\ \text{A} & & \text{A} \end{smallmatrix}$  has priority over  $\equiv\text{A}$ . Actually, both atoms of

a multiple bond are duplicated, or triplicated, so that  $\text{C}=\text{O}$  is treated as  $\begin{smallmatrix} \text{C}-\text{O} \\ | \quad | \\ \text{O} \quad \text{C} \end{smallmatrix}$ , that

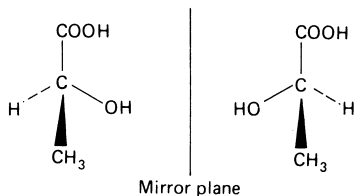
is  $\begin{smallmatrix} \text{C}-\text{O} \\ | \\ \text{O} \end{smallmatrix}$  and  $\begin{smallmatrix} \text{O}-\text{C} \\ | \\ \text{C} \end{smallmatrix}$ , and  $\text{C}\equiv\text{N}$  is treated as  $\begin{smallmatrix} \text{C} & & \text{N} \\ / \quad & \backslash & / \\ (\text{N}) & (\text{N}) & (\text{C}) & (\text{N}) \end{smallmatrix}$ . A phenyl carbon

becomes  $\begin{smallmatrix} \text{CH} \\ | \\ -\text{C} & & \text{C} \\ | \quad \backslash \\ \text{CH} \end{smallmatrix}$ . Only the double-bonded atoms themselves are duplicated, not the atoms or

groups attached to them. The duplicated atoms (or phantom atoms) may be considered as carrying atomic number zero. For example, among the groups OH, CHO,  $\text{CH}_2\text{OH}$ , and H, the OH group has the highest priority, and the C(O, O, H) of CHO takes priority over the C(O, H, H) of  $\text{CH}_2\text{OH}$ .

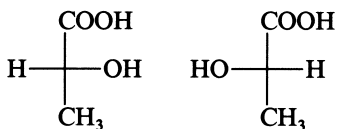
**1.1.4.4 Chirality and Optical Activity.** A compound is chiral (the term *dissymmetric* was formerly used) if it is not superimposable on its mirror image. A chiral compound does not have a plane of symmetry. Each chiral compound possesses one (or more) of three types of chiral element, namely, a chiral center, a chiral axis, or a chiral plane.

**Chiral Center.** The chiral center, which is the chiral element most commonly met, is exemplified by an asymmetric carbon with a tetrahedral arrangement of ligands about the carbon. The ligands comprise four different atoms or groups. One “ligand” may be a lone pair of electrons; another, a phantom atom of atomic number zero. This situation is encountered in sulfoxides or with a nitrogen atom. Lactic acid is an example of a molecule with an asymmetric (chiral) carbon. (See Fig. 1.13b.)



**FIGURE 1.13** Asymmetric (chiral) carbon in the lactic acid molecule.

A simpler representation of molecules containing asymmetric carbon atoms is the Fischer projection, which is shown here for the same lactic acid configurations. A Fischer projection involves



drawing a cross and attaching to the four ends the four groups that are attached to the asymmetric carbon atom. The asymmetric carbon atom is understood to be located where the lines cross. The horizontal lines are understood to represent bonds coming toward the viewer out of the plane of the paper. The vertical lines represent bonds going away from the viewer behind the plane of the paper as if the vertical line were the side of a circle. The principal chain is depicted in the vertical direction; the lowest-numbered (locant) chain member is placed at the top position. These formulas may be moved sideways or rotated through  $180^\circ$  in the plane of the paper, but they may not be removed from the plane of the paper (i.e., rotated through  $90^\circ$ ). In the latter orientation it is essential to use thickened lines (for bonds coming toward the viewer) and dashed lines (for bonds receding from the viewer) to avoid confusion.

**Enantiomers.** Two nonsuperimposable structures that are mirror images of each other are known as *enantiomers*. Enantiomers are related to each other in the same way that a right hand is related to a left hand. Except for the direction in which they rotate the plane of polarized light, enantiomers are identical in all physical properties. Enantiomers have identical chemical properties except in their reactivity toward optically active reagents.

Enantiomers rotate the plane of polarized light in opposite directions but with equal magnitude. If the light is rotated in a clockwise direction, the sample is said to be dextrorotatory and is designed as (+). When a sample rotates the plane of polarized light in a counterclockwise direction, it is said to be levorotatory and is designed as (–). Use of the designations *d* and *l* is discouraged.

**Specific Rotation.** Optical rotation is caused by individual molecules of the optically active compound. The amount of rotation depends upon how many molecules the light beam encounters in passing through the tube. When allowances are made for the length of the tube that contains the sample and the sample concentration, it is found that the amount of rotation, as well as its direction, is a characteristic of each individual optically active compound.

Specific rotation is the number of degrees of rotation observed if a 1-dm tube is used and the compound being examined is present to the extent of 1 g per 100 mL. The density for a pure liquid replaces the solution concentration.

$$\text{Specific rotation} = [\alpha] = \frac{\text{observed rotation (degrees)}}{\text{length (dm)} \times (\text{g}/100 \text{ mL})}$$

The temperature of the measurement is indicated by a superscript and the wavelength of the light employed by a subscript written after the bracket; for example,  $[\alpha]_{590}^{20}$  implies that the measurement was made at 20°C using 590-nm radiation.

**Optically Inactive Chiral Compounds.** Although chirality is a necessary prerequisite for optical activity, chiral compounds are not necessarily optically active. With an equal mixture of two enantiomers, no net optical rotation is observed. Such a mixture of enantiomers is said to be *racemic* and is designated as ( $\pm$ ) and not as *dl*. Racemic mixtures usually have melting points higher than the melting point of either pure enantiomer.

A second type of optically inactive chiral compounds, *meso* compounds, will be discussed in the next section.

**Multiple Chiral Centers.** The number of stereoisomers increases rapidly with an increase in the number of chiral centers in a molecule. A molecule possessing two chiral atoms should have four optical isomers, that is, four structures consisting of two pairs of enantiomers. However, if a compound has two chiral centers but both centers have the same four substituents attached, the total number of isomers is three rather than four. One isomer of such a compound is not chiral because it is identical with its mirror image; it has an internal mirror plane. This is an example of a diastereomer. The achiral structure is denoted as a *meso* compound. Diastereomers have different physical and chemical properties from the optically active enantiomers. Recognition of a plane of symmetry is usually the easiest way to detect a *meso* compound. The stereoisomers of tartaric acid are examples of compounds with multiple chiral centers (see Fig. 1.14), and one of its isomers is a *meso* compound.

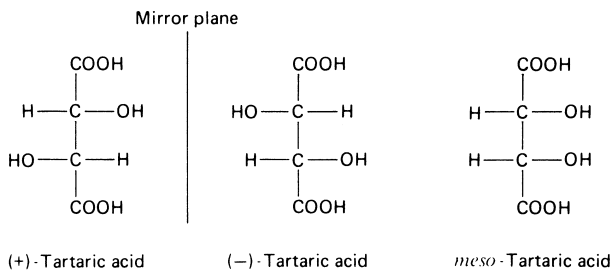
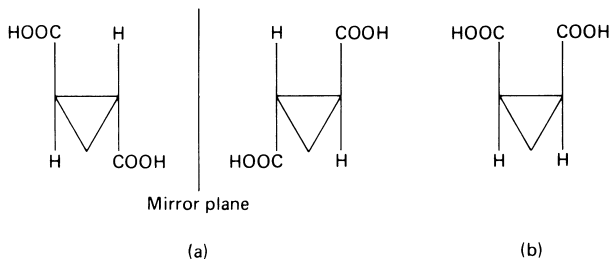


FIGURE 1.14 Isomers of tartaric acid.

When the asymmetric carbon atoms in a chiral compound are part of a ring, the isomerism is more complex than in acyclic compounds. A cyclic compound which has two different asymmetric carbons with different sets of substituent groups attached has a total of  $2^2 = 4$  optical isomers: an enantiomeric pair of *cis* isomers and an enantiomeric pair of *trans* isomers. However, when the two asymmetric centers have the same set of substituent groups attached, the *cis* isomer is a *meso* compound and only the *trans* isomer is chiral. (See Fig. 1.15.)

**Torsional Asymmetry.** Rotation about single bonds of most acyclic compounds is relatively free at ordinary temperatures. There are, however, some examples of compounds in which nonbonded



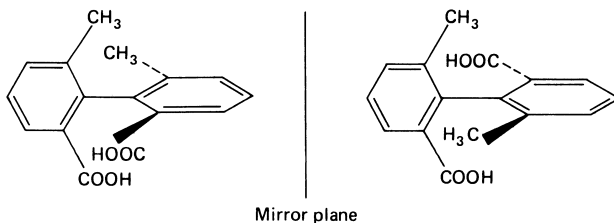
**FIGURE 1.15** Isomers of cyclopropane-1,2-dicarboxylic acid. (a) *Trans* isomer; (b) *meso* isomer.

interactions between large substituent groups inhibit free rotation about a sigma bond. In some cases these compounds can be separated into pairs of enantiomers.

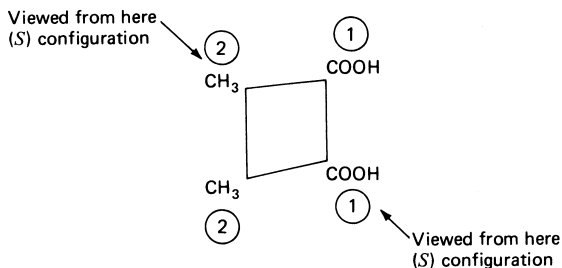
A *chiral axis* is present in chiral biaryl derivatives. When bulky groups are located at the *ortho* positions of each aromatic ring in biphenyl, free rotation about the single bond connecting the two rings is inhibited because of torsional strain associated with twisting rotation about the central single bond. Interconversion of enantiomers is prevented (see Fig. 1.16).

For compounds possessing a chiral axis, the structure can be regarded as an elongated tetrahedron to be viewed along the axis. In deciding upon the absolute configuration it does not matter from which end it is viewed; the nearer pair of ligands receives the first two positions in the order of precedence (see Fig. 1.17). For the meaning of (*S*), see the discussion under Absolute Configuration on p. 1.49.

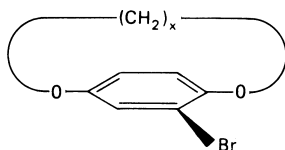
A *chiral plane* is exemplified by the plane containing the benzene ring and the bromine and oxygen atoms in the chiral compound shown in Fig. 1.18. Rotation of the benzene ring around the oxygen-to-ring single bonds is inhibited when  $x$  is small (although no critical size can be reasonably established).



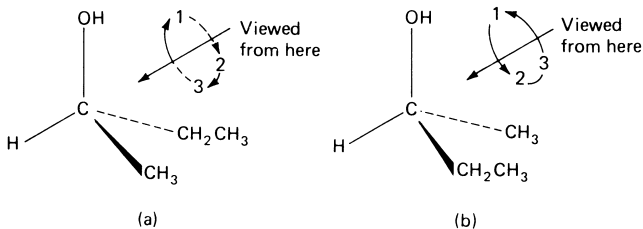
**FIGURE 1.16** Isomers of biphenyl compounds with bulky groups attached at the *ortho* positions.



**FIGURE 1.17** Example of a chiral axis.



**FIGURE 1.18** Example of a chiral plane.



**FIGURE 1.19** Viewing angle as a means of designating the absolute configuration of compounds with a chiral axis. (a) (*R*)-2-Butanol (sequence clockwise); (b) (*S*)-2-butanol (sequence counterclockwise).

**Absolute Configuration.** The terms absolute stereochemistry and absolute configuration are used to describe the three-dimensional arrangement of substituents around a chiral element. A general system for designating absolute configuration is based upon the priority system and sequence rules. Each group attached to a chiral center is assigned a number, with number one the highest-priority group. For example, the groups attached to the chiral center of 2-butanol (see Fig. 1.19) are assigned these priorities: 1 for OH, 2 for CH<sub>2</sub>CH<sub>3</sub>, 3 for CH<sub>3</sub>, and 4 for H. The molecule is then viewed from the side opposite the group of lowest priority (the hydrogen atom), and the arrangement of the remaining groups is noted. If, in proceeding from the group of highest priority to the group of second priority and thence to the third, the eye travels in a clockwise direction, the configuration is specified *R* (from the Latin *rectus*, “right”); if the eye travels in a counterclockwise direction, the configuration is specified *S* (from the Latin *sinister*, “left”). The complete name includes both configuration and direction of optical rotation, as for example, (*S*)-(+)-2-butanol.

The relative configurations around the chiral centers of many compounds have been established. One optically active compound is converted to another by a sequence of chemical reactions which are stereospecific; that is, each reaction is known to proceed spatially in a specific way. The configuration of one chiral compound can then be related to the configuration of the next in sequence. In order to establish absolute configuration, one must carry out sufficient stereospecific reactions to relate a new compound to another of known absolute configuration. Historically the configuration of **D**-(+)-2,3-dihydroxypropanal has served as the standard to which all configuration has been compared. The absolute configuration assigned to this compound has been confirmed by an X-ray crystallographic technique.

### 1.1.5 Chemical Abstracts Indexing System

When compounds of complex structure are considered, the number of name possibilities grows rapidly. To avoid having index entries for all possible names, Chemical Abstracts Service has developed what might be called the principle of inversion. The indexing system employs inverted

entries to bring together related compounds in an alphabetically arranged index. The *index heading parent* from the Chemical Substance Index appears in the Formula Index in lightface before the “comma of inversion.” The *substituents* follow the “comma of inversion” in alphabetical order. Any *name modification* appears on a separate line. If necessary, the chemical description is completed by citation of an associated ion, a functional derivative, a “salt with” or “compound with” term, and/or a stereochemical descriptor.

Quite naturally there is a certain amount of arbitrariness in this system, although the IUPAC nomenclature is followed. The preferred *Chemical Abstracts* index names for chemical substances have been, with very few exceptions, continued unchanged (since 1972) as set forth in the *Ninth Collective Index Guide* and in a journal article.\* Any revisions appear in the updated *Index Guide*; new editions appear at 18-month intervals. Appendix VI is of particular interest to chemists. Reprints of the Appendix may be purchased from Chemical Abstracts Service, Marketing Division, P.O. Box 3012, Columbus, Ohio 43210.

---

\* *J. Chem. Doc.* **14**(1):3–15 (1974).



**TABLE 1.13** Names and Formulas of Organic Radicals

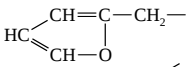
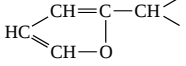
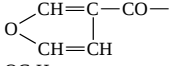
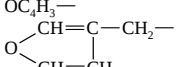
For more comprehensive lists, see the various lists of radicals given in the subject indexes of the annual and decennial indexes of Chemical Abstracts.

| Name                                                                        | Formula                                          | Name                                              | Formula                           |
|-----------------------------------------------------------------------------|--------------------------------------------------|---------------------------------------------------|-----------------------------------|
| Acenaphthenyl                                                               | $C_{12}H_9-$                                     | Azido                                             | $N_3-$                            |
| Acenaphthenylene                                                            | $-C_{12}H_8-$                                    | Azino                                             | $=N-N=$                           |
| Acenaphthenylidene                                                          | $C_{12}H_8=$                                     | Azo                                               | $-N=N-$                           |
| Acetamido                                                                   | $CH_3-CO-NH-$                                    | Azoxy                                             | $-N(O)-N-$                        |
| Acetimidoyl                                                                 | $CH_3C(=NH)-$                                    | Azulenyl                                          | $C_{10}H_7-$                      |
| Acetoacetyl                                                                 | $CH_3-CO-CH_2-CO-$                               | Benzamido                                         | $C_6H_5-CO-NH-$                   |
| Acetohydrazonoyl                                                            | $CH_3-C(=NNH_2)-$                                | Benzeneazo                                        | $C_6H_5-N=N-$                     |
| Acetohydroximoyl                                                            | $CH_3-C(=NOH)-$                                  | Benzeneazoxy                                      | $C_6H_5-N_2O-$                    |
| Acetonyl                                                                    | $CH_3-CO-CH_2-$                                  | 1,2-Benzenedicarbonyl,<br>see Phthaloyl           |                                   |
| Acetonylidene                                                               | $CH_3-CO-CH=$                                    | 1,3-Benzenedicarbonyl (or<br>isophthaloyl)        | $-CO-C_6H_4-CO-$ ( <i>m</i> -)    |
| Acetoxyl                                                                    | $CH_3-CO-O-$                                     | 1,4-Benzenedicarbonyl (or<br>terephthaloyl)       | $-CO-C_6H_4-CO-$ ( <i>p</i> -)    |
| Acetyl (not ethanoyl)                                                       | $CH_3-CO-$                                       | Benzenesulfinyl                                   | $C_6H_5-SO-$                      |
| Acetylamino                                                                 | $CH_3-CO-NH-$                                    | Benzenesulfonamido                                | $C_6H_5-SO_2-NH-$                 |
| Acetylhydrazino                                                             | $CH_3-CO-NH-NH-$                                 | Benzenesulfonyl                                   | $C_6H_5-SO_2-$                    |
| Acetylmino                                                                  | $CH_3-CO-N=$                                     | Benzenesulfonylamino                              | $C_6H_5-SO_2-NH-$                 |
| Acridinyl (from acridine)                                                   | $NC_{13}H_8-$                                    | Benzenetriyl                                      | $C_6H_3-$                         |
| Acroyloyl (or propenoyl)                                                    | $CH_2=CH-CO-$                                    | Benzhydryl (or diphenyl-<br>methyl)               | $(C_6H_5)_2CH-$                   |
| Adipoyl (or hexanedioyl)                                                    | $-CO-[CH_2]_4-CO-$                               | Benzidino                                         | $p\text{-}H_2N-C_6H_4-C_6H_4-NH-$ |
| Alanyl                                                                      | $CH_3-CH(NH_2)-CO-$                              | Benziloyl (or 2-hydroxy-<br>2,2-diphenylethanoyl) | $(C_6H_5)_2C(OH)-CO-$             |
| $\beta$ -Alanyl                                                             | $H_2N-CH_2-CH_2-CO-$                             | Benzimidazolyl                                    | $N_2C_7H_5-$                      |
| Allyl (or 2-propenyl)                                                       | $CH_2=CH-CH_2-$                                  | Benzimidoyl                                       | $C_6H_5-C(=NH)-$                  |
| Allylidene                                                                  | $CH_2=CH-CH=$                                    | Benzofuranyl                                      | $OC_8H_5-$                        |
| Allyloxy                                                                    | $CH_2=CH-CH_2-O-$                                | Benzopyranyl                                      | $OC_9H_7-$                        |
| Amidino                                                                     | $H_2N-N-C(=NH)-$                                 | Benzoquinonyl (1,2- or<br>1,4-)                   | $(O=)_2C_6H_3-$                   |
| Amino                                                                       | $H_2N-$                                          | Benzo[ <i>b</i> ]thienyl                          | $SC_6H_5-$                        |
| Aminomethyleneamino                                                         | $H_2N-CH=N-$                                     | Benzoyl                                           | $C_6H_5-CO-$                      |
| Aminooxy                                                                    | $H_2N-O-$                                        | Benzoylamino                                      | $C_6H_5-CO-NH-$                   |
| Ammonio                                                                     | $^+H_3N-$                                        | Benzoylhydrazino                                  | $C_6H_5-CO-NH-NH-$                |
| Amyl, see Pentyl                                                            |                                                  | Benzoylimino                                      | $C_6H_5-CO-N=$                    |
| Anilino                                                                     | $C_6H_5-NH-$                                     | Benzoyloxy                                        | $C_6H_5-CO-O-$                    |
| Anisidino ( <i>o</i> -, <i>m</i> -, or<br><i>p</i> -)                       | $CH_3O-C_6H_4-NH-$                               | Benzyl                                            | $C_6H_5-CH_2-$                    |
| Anisoyl ( <i>o</i> -, <i>m</i> -, or<br><i>p</i> -; or methoxyben-<br>zoyl) | $CH_3O-C_6H_4-CO-$                               | Benzylidene                                       | $C_6H_5-CH=$                      |
| Anthraniloyl                                                                | <i>o</i> - $NH_2-C_6H_4-CO-$                     | Benzylidyne                                       | $C_6H_5-C\equiv$                  |
| Anthryl (from anthracene)                                                   | $C_{14}H_9-$                                     | Benzylloxy                                        | $C_6H_5-CH_2-O-$                  |
| Anthrylene                                                                  | $-C_{14}H_8-$                                    | Benzylloxycarbonyl                                | $C_6H_5-CH_2-O-CO-$               |
| Arginyl                                                                     | $H_2N-C(=NH)-NH-$<br>$[CH_2]_3-CH(NH)-$<br>$CO-$ | Benzylthio                                        | $C_6H_5-CH_2-S-$                  |
| Asparaginyll                                                                | $H_2N-CO-CH_2-$<br>$CH(NH_2)-CO-$                | Biphenylenyl                                      | $C_{12}H_7-$                      |
| Aspartoyl                                                                   | $-CO-CH_2-$<br>$CH(NH_2)-CO-$                    | Biphenyllyl                                       | $C_6H_5-C_6H_4-$                  |
| $\alpha$ -Aspartyl                                                          | $HO_2C-CH_2CH(NH_2)-$                            | Bornenyl                                          | $C_{10}H_{15}-$                   |
| Atropoyl (or 2-phenylpro-<br>penoyl)                                        | $C_6H_5-C(=CH_2)-CO-$                            | Bornyl (not camphyl or<br>bornyllyl)              | $C_{10}H_{17}-$                   |
| Azelaoyl, see Nonane-<br>dioyl                                              |                                                  | Bromo                                             | $Br-$                             |
|                                                                             |                                                  | Bromoformyl                                       | $Br-CO-$                          |

**TABLE 1.13** Names and Formulas of Organic Radicals (*Continued*)

| Name                                                                 | Formula                                                             | Name                                             | Formula                                                                                                                     |
|----------------------------------------------------------------------|---------------------------------------------------------------------|--------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| Bromonio                                                             | $^+\text{HBr}-$                                                     | Cinnamoyl ( <i>or 3-phenyl-propenoyl</i> )       | $\text{C}_6\text{H}_5-\text{CH}=\text{CH}-\text{CO}-$                                                                       |
| Butadienyl (1,3- shown)                                              | $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}-$                        | Cinnamyl                                         | $\text{C}_6\text{H}_5-\text{CH}=\text{CH}-\text{CH}_2-$                                                                     |
| Butanedioyl, <i>see</i> Succinyl                                     |                                                                     | Cinnamylidene                                    | $\text{C}_6\text{H}_5-\text{CH}=\text{CH}-\text{CH}=\text{CH}-$                                                             |
| Butanediylidene                                                      | $=\text{CH}-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}=\text{CH}-$     | Citraconoyl ( <i>unsubstituted only</i> )        | $\text{HC}-\text{CO}-$<br>$\text{CH}_3-\text{C}-\text{CO}-$                                                                 |
| Butanediylidene                                                      | $\equiv\text{C}-\text{CH}_2-\text{CH}_2-\text{C}\equiv$             | Crotonoyl                                        | $\text{CH}_3-\text{CH}=\text{CH}-\text{CO}-$<br>( <i>trans</i> )                                                            |
| Butanediylidene                                                      |                                                                     | Crotyl, <i>see</i> 2-Butenyl                     |                                                                                                                             |
| Butanoyl, <i>see</i> Butyryl                                         |                                                                     | Cumenyl ( <i>o</i> -, <i>m</i> -, or <i>p</i> -) | $(\text{CH}_3)_2\text{CH}-\text{C}_6\text{H}_4-$                                                                            |
| <i>cis</i> -Butenedioidyl, <i>see</i> Maleoyl                        |                                                                     | Cyanato                                          | $\text{NCO}-$                                                                                                               |
| <i>trans</i> -Butenedioidyl, <i>see</i> Fumaroyl                     |                                                                     | Cyano                                            | $\text{NC}-$                                                                                                                |
| Butenyl, <i>see</i> Butenyl                                          |                                                                     | Cyclobutyl                                       | $\text{C}_4\text{H}_7-$                                                                                                     |
| 2-Butenyl ( <i>not</i> crotyl)                                       | $\text{CH}_3-\text{CH}=\text{CH}-\text{CH}_2-$                      | Cycloheptyl                                      | $\text{C}_7\text{H}_{13}-$                                                                                                  |
| 2-Butenylene                                                         | $-\text{CH}_2-\text{CH}=\text{CH}-$<br>$\text{CH}_2-$               | Cyclohexadienyl (2,4- shown)                     | $\text{CH}=\text{CH}-\text{CH}-$<br>$\text{CH}=\text{CH}-\text{CH}_2$                                                       |
| Butenylidene (2- shown)                                              | $\text{CH}_3\text{CH}=\text{CH}-\text{CH}=\text{CH}-$               | Cyclohexadienylidene (2,4- shown)                | $\text{CH}-\text{CH}_2-\text{C}$<br>$\text{CH}=\text{CH}-\text{CH}$                                                         |
| Butenylidyne (2- shown)                                              | $\text{CH}_3-\text{CH}=\text{CH}-\text{C}\equiv$                    | Cyclohexanecarbonyl                              | $\text{C}_6\text{H}_{11}-\text{CO}-$                                                                                        |
| Butoxy                                                               | $\text{CH}_3-[\text{CH}_2]_3-\text{O}-$                             | Cyclohexanecarbothioidyl                         | $\text{C}_6\text{H}_{11}-\text{CS}-$                                                                                        |
| <i>sec</i> -Butoxy ( <i>unsubstituted only</i> )                     | $\text{C}_2\text{H}_5-\text{CH}(\text{CH}_3)-\text{O}-$             | Cyclohexanecarboxamido                           | $\text{C}_6\text{H}_{11}-\text{CO}-\text{NH}-$                                                                              |
| <i>tert</i> -Butoxy ( <i>unsubstituted only</i> )                    | $(\text{CH}_3)_3\text{C}-\text{O}-$                                 | Cyclohexanecarboximidoyl                         | $\text{C}_6\text{H}_{11}-\text{C}(=\text{NH})-$                                                                             |
| Butyl                                                                | $\text{CH}_3-[\text{CH}_2]_3-$ or $\text{C}_4\text{H}_9-$           | Cyclohexenyl                                     | $\text{C}_6\text{H}_9-$                                                                                                     |
| <i>sec</i> -Butyl ( <i>unsubstituted only</i> )                      | $\text{C}_2\text{H}_5-\text{CH}(\text{CH}_3)-$                      | 2-Cyclohexenylidene                              | $\text{CH}=\text{CH}-\text{C}$<br>$\text{H}_2\text{C}-\text{CH}_2-\text{CH}_2$                                              |
| <i>tert</i> -Butyl ( <i>unsubstituted only</i> )                     | $(\text{CH}_3)_3\text{C}-$                                          | Cyclohexyl                                       | $\text{C}_6\text{H}_{11}-$                                                                                                  |
| Butylidene                                                           | $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}-$          | Cyclohexylcarbonyl                               | $\text{C}_6\text{H}_{11}-\text{CO}-$                                                                                        |
| <i>sec</i> -Butylidene ( <i>unsubstituted only</i> )                 | $\text{C}_2\text{H}_5\text{C}(\text{CH}_3)=$                        | Cyclohexylene                                    | $-\text{C}_6\text{H}_{10}-$                                                                                                 |
| Butylidyne                                                           | $\text{CH}_3-[\text{CH}_2]_2-\text{C}\equiv$                        | Cyclohexylidene                                  | $\text{CH}_2-\text{CH}_2-\text{C}$<br>$\text{CH}_2-\text{CH}_2-\text{CH}_2$                                                 |
| Butyryl ( <i>or</i> butanoyl)                                        | $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CO}-$                    | Cyclohexylthiocarbonyl                           | $\text{C}_6\text{H}_{11}-\text{CS}-$                                                                                        |
| Camphoroyl                                                           | $\text{C}_{10}\text{H}_{14}\text{O}_2-$                             | Cyclopentadienyl                                 | $\text{C}_5\text{H}_5-$                                                                                                     |
| Carbamoyl                                                            | $\text{H}_2\text{N}-\text{CO}-$                                     | Cyclopentadienylidene                            | $\text{CH}=\text{CH}-\text{CH}=\text{CH}-\text{C}=\text{CH}-$                                                               |
| Carbazoyl                                                            | $\text{NC}_{12}\text{H}_8-$                                         | Cyclopenta[ <i>a</i> ]phenanthryl                | $\text{C}_{17}\text{H}_{17}-$                                                                                               |
| Carbazoyl                                                            | $\text{H}_2\text{N}-\text{NH}-\text{CO}-$                           | 1,2-Cyclopentenophenanthryl                      | $\text{C}_{17}\text{H}_{11}-$                                                                                               |
| Carbonimidoyl                                                        | $-\text{C}(=\text{NH})-$                                            | Cyclopentenyl                                    | $\text{C}_5\text{H}_7-$                                                                                                     |
| Carbonohydrazido ( <i>preferred to carbohydrazido or carbazido</i> ) | $\text{H}_2\text{N}-\text{NH}-\text{CO}-\text{NH}-$<br>$\text{NH}-$ | Cyclopentyl                                      | $\text{C}_5\text{H}_9-$                                                                                                     |
| Carbonyl                                                             | $-\text{CO}-$ or $=\text{C}(\text{O})$                              | Cyclopentylene                                   | $-\text{C}_5\text{H}_8-$                                                                                                    |
| Carbonyldioxy                                                        | $-\text{O}-\text{CO}-\text{O}-$                                     | Cyclopropyl                                      | $\text{C}_3\text{H}_5-$                                                                                                     |
| Carboxy                                                              | $\text{HO}_2\text{C}-$                                              | Cysteinyl                                        | $\text{HS}-\text{CH}_2-\text{CH}(\text{NH}_2)-$<br>$\text{CO}-$                                                             |
| Carboxylato                                                          | $-\text{O}_2\text{C}-$                                              | Cystyl                                           | $-\text{CO}-\text{CH}(\text{NH}_2)-$<br>$\text{CH}_2-\text{S}-\text{S}-\text{CH}_2-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$ |
| Chloro                                                               | $\text{Cl}-$                                                        | Decanedioyl                                      | $-\text{CO}-[\text{CH}_2]_8-\text{CO}-$                                                                                     |
| Chlorocarbonyl, <i>see</i> Chloroformyl                              |                                                                     | Decanoyl                                         | $\text{CH}_3-[\text{CH}_2]_8-\text{CO}-$                                                                                    |
| Chloroformyl                                                         | $\text{Cl}-\text{C}(\text{O})-$                                     | Decyl                                            | $\text{CH}_3-[\text{CH}_2]_9-$                                                                                              |
| Chlorosyl                                                            | $\text{OCl}-$                                                       | Diacetoxiyodo                                    | $(\text{CH}_3-\text{CO}-\text{O})_2\text{I}-$                                                                               |
| Chlorothio                                                           | $\text{ClS}-$                                                       | Diacetylamino                                    | $(\text{CH}_3-\text{CO})_2\text{N}-$                                                                                        |
| Chloryl                                                              | $\text{O}_2\text{Cl}-$                                              | Diaminomethyleneamino                            | $(\text{NH}_2)_2\text{C}=\text{N}-$                                                                                         |

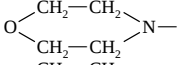
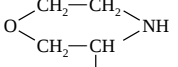
**TABLE 1.13** Names and Formulas of Organic Radicals (*Continued*)

| Name                                                    | Formula                                                                          | Name                                                                       | Formula                                                                                        |
|---------------------------------------------------------|----------------------------------------------------------------------------------|----------------------------------------------------------------------------|------------------------------------------------------------------------------------------------|
| Diazo                                                   | $\equiv \text{N}_2$                                                              | Fluorenyl                                                                  | $\text{C}_{13}\text{H}_9-$                                                                     |
| Diazoamino                                              | $-\text{N}=\text{N}-\text{NH}-$                                                  | Fluoro                                                                     | $\text{F}-$                                                                                    |
| Dibenzoylamino                                          | $(\text{C}_6\text{H}_5-\text{CO})_2\text{N}-$                                    | Fluoroformyl                                                               | $\text{F}-\text{CO}-$                                                                          |
| Dichloroiodo                                            | $\text{Cl}_2\text{I}-$                                                           | Formamido                                                                  | $\text{OCH}-\text{NH}-$                                                                        |
| Diethylamino                                            | $(\text{C}_2\text{H}_5)_2\text{N}-$                                              | Formimidoyl                                                                | $\text{CH}(=\text{NH})-$                                                                       |
| 3,4-Dihydroxybenzoyl, <i>see</i><br>Protocatechuoyl     |                                                                                  | Formyl ( <i>not methanoyl</i> )                                            | $\text{OCH}-$ or $-\text{C}(\text{O})\text{H}$                                                 |
| 2,3-Dihydroxybutanedioyl,<br><i>see</i> Tartaroyl       |                                                                                  | Formylamino                                                                | $\text{H}-\text{CO}-\text{NH}-$                                                                |
| Dihydroxyiodo                                           | $(\text{HO})_2\text{I}-$                                                         | Formylimino                                                                | $\text{H}-\text{CO}-\text{N}=\text{}$                                                          |
| 2,3-Dihydroxypropanoyl,<br><i>see</i> Glyceroyl         |                                                                                  | Formyloxy                                                                  | $\text{H}-\text{CO}-\text{O}-$                                                                 |
| 3,4-Dimethoxybenzoyl,<br><i>see</i> Veratroyl           |                                                                                  | Fumaroyl ( <i>or trans-butene-</i><br><i>diolyl</i> )                      | $-\text{CO}-\text{CH}=\text{CH}-\text{CO}-$<br>( <i>trans</i> )                                |
| 3,4-Dimethoxyphenethyl                                  |                                                                                  | Furancarbonyl, <i>see</i> Furoyl                                           |                                                                                                |
| 3,4-Dimethoxyphenylace-<br>tyl                          | 3,4-<br>$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{CH}_2\text{CH}-$       | Furfuryl (2- <i>only</i> ; <i>pre-</i><br><i>ferred to 2-furylmethyl</i> ) |               |
| 3,4-Dimethoxyphenylace-<br>tyl                          | 3,4-<br>$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{CH}_2\text{CO}-$       | Furfurylidene (2- <i>only</i> )                                            |               |
| Dimethylamino                                           | $(\text{CH}_3)_2\text{N}-$                                                       | Furoyl (3- <i>shown</i> ; <i>pre-</i><br><i>ferred to furancarbonyl</i> )  |               |
| Dimethylbenzoyl                                         | $(\text{CH}_3)_2\text{C}_6\text{H}_4-\text{CO}-$                                 | Furyl                                                                      | $\text{OC}_4\text{H}_3-$                                                                       |
| Dioxy                                                   | $-\text{O}-\text{O}-$                                                            | 3-Furylmethyl                                                              |               |
| Diphenylamino                                           | $(\text{C}_6\text{H}_5)_2\text{N}-$                                              |                                                                            |                                                                                                |
| Diphenylmethylene                                       | $(\text{C}_6\text{H}_5)_2\text{C}=\text{}$                                       |                                                                            |                                                                                                |
| Dithio                                                  | $-\text{S}-\text{S}-$                                                            | Galloyl ( <i>or 3,4,5-trihy-</i><br><i>droxybenzoyl</i> )                  | 3,4,5-(HO) $_3\text{C}_6\text{H}_2-\text{CO}-$                                                 |
| Diethiocarboxy                                          | $\text{HSSC}-$                                                                   | Geranyl ( <i>from geraniol</i> )                                           | $\text{C}_{10}\text{H}_{17}-$                                                                  |
| Dithiosulfo                                             | $\text{HOS}_2-$                                                                  | Glutamyl                                                                   | $\text{H}_2\text{N}-\text{CO}-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$ |
| Dodecanoyl                                              | $\text{CH}_3[\text{CH}_2]_{10}-\text{CO}-$                                       |                                                                            | $-\text{CO}-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$                   |
| Dodecyl                                                 | $\text{CH}_3[\text{CH}_2]_{11}-$                                                 | $\alpha$ -Glutamyl                                                         | $\text{HOOC}[\text{CH}_2]_2\text{CH}(\text{NH}_2)-$<br>$\text{CO}-$                            |
| Elaidoyl ( <i>or trans-9-octa-</i><br><i>decenoyl</i> ) | $\text{CH}_3[\text{CH}_2]_7\text{CH}=\text{CH}-$<br>$[\text{CH}_2]_7-\text{CO}-$ | $\gamma$ -Glutamyl                                                         | $\text{HOOC}-\text{CH}(\text{NH}_2)-$<br>$[\text{CH}_2]_2-\text{CO}-$                          |
| Epidioxy (as a bridge)                                  | $-\text{O}-\text{O}-$                                                            | Glutaryl ( <i>or pentanedioyl</i> )                                        | $-\text{CO}-[\text{CH}_2]_3-\text{CO}-$                                                        |
| Epidiseleno (as a bridge)                               | $-\text{Se}-\text{Se}-$                                                          | Glyceroyl ( <i>or 2,3- dihy-</i><br><i>droxypropanoyl</i> )                | $\text{HO}-\text{CH}_2-\text{CH}(\text{OH})-$<br>$\text{CO}-$                                  |
| Epidithio (as a bridge)                                 | $-\text{S}-\text{S}-$                                                            | Glycoloyl ( <i>or hydroxy-</i><br><i>ethanoyl</i> )                        | $\text{HO}-\text{CH}_2-\text{CO}-$                                                             |
| Epimino (as a bridge)                                   | $-\text{NH}-$                                                                    | Glycyl                                                                     | $\text{H}_2\text{N}-\text{CH}_2-\text{CO}-$                                                    |
| Episeleno (as a bridge)                                 | $-\text{Se}-$                                                                    | Glycylamino                                                                | $\text{H}_2\text{N}-\text{CH}_2-\text{CO}-\text{NH}-$                                          |
| Epithio (as a bridge)                                   | $-\text{S}-$                                                                     | Glyoxyloyl                                                                 | $\text{OHC}-\text{CO}-$                                                                        |
| Epoxy (as a bridge)                                     | $-\text{O}-$                                                                     | Guanidino                                                                  | $\text{H}_2\text{N}-\text{C}(=\text{NH})-\text{NH}-$                                           |
| Ethanesulfonamide                                       | $\text{C}_2\text{H}_5-\text{SO}_2-\text{NH}-$                                    | Guanyl, <i>see</i> Amidino                                                 |                                                                                                |
| Ethanoyl, <i>see</i> Acetyl                             |                                                                                  | Heptanamido                                                                | $\text{CH}_3-[\text{CH}_2]_5-\text{CO}-\text{NH}-$<br>$-\text{CO}-[\text{CH}_2]_5-\text{CO}-$  |
| Ethenyl, <i>see</i> Vinyl                               |                                                                                  | Heptanedioyl                                                               | $\text{CH}_3-[\text{CH}_2]_5-\text{CO}-$                                                       |
| Ethoxalyl                                               | $\text{C}_2\text{H}_5-\text{OOC}-\text{CO}-$                                     | Heptanoyl                                                                  | $\text{CH}_3-[\text{CH}_2]_5-\text{CH}_2-$                                                     |
| Ethoxy                                                  | $\text{C}_2\text{H}_5-\text{O}-$                                                 | Heptyl                                                                     | $\text{CH}_3-[\text{CH}_2]_{14}-\text{CO}-$                                                    |
| Ethoxycarbonyl                                          | $\text{C}_2\text{H}_5-\text{O}-\text{CO}-$                                       | Hexadecanoyl                                                               | $\text{CH}_3-[\text{CH}_2]_{14}-\text{CO}-$                                                    |
| Ethyl                                                   | $\text{C}_2\text{H}_5-$ or $\text{CH}_3-\text{CH}_2-$                            | Hexadecyl                                                                  | $\text{CH}_3-[\text{CH}_2]_{14}-\text{CH}_2-$<br>$-\text{CO}-$                                 |
| Ethylamino                                              | $\text{C}_2\text{H}_5-\text{NH}-$                                                | Hexamethylene                                                              | $-\text{CH}_2]_6-$                                                                             |
| Ethylene                                                | $-\text{CH}_2-\text{CH}_2-$                                                      | Hexanamido                                                                 | $\text{CH}_3-[\text{CH}_2]_4-\text{CO}-\text{NH}-$<br>$-\text{CO}-[\text{CH}_2]_4-\text{CO}-$  |
| Ethylenedioxy                                           | $-\text{O}-\text{CH}_2-\text{CH}_2-\text{O}-$                                    | Hexanedioyl ( <i>or adipoyl</i> )                                          |                                                                                                |
| Ethylidene                                              | $\text{CH}_3-\text{CH}=\text{}$                                                  |                                                                            |                                                                                                |
| Ethylidyne                                              | $\text{CH}_3-\text{C}\equiv$                                                     |                                                                            |                                                                                                |
| Ethylsulfonylamino                                      | $\text{C}_2\text{H}_5-\text{SO}_2-\text{NH}-$                                    |                                                                            |                                                                                                |
| Ethylthio                                               | $\text{C}_2\text{H}_5-\text{S}-$                                                 |                                                                            |                                                                                                |
| Ethynyl                                                 | $\text{HC}\equiv\text{C}-$                                                       |                                                                            |                                                                                                |
| Ethynylene                                              | $-\text{C}\equiv\text{C}-$                                                       |                                                                            |                                                                                                |
| Fluoranthenyl                                           | $\text{C}_{16}\text{H}_9-$                                                       |                                                                            |                                                                                                |

**TABLE 1.13** Names and Formulas of Organic Radicals (*Continued*)

| Name                                                 | Formula                                                                 | Name                                                           | Formula                                                                         |
|------------------------------------------------------|-------------------------------------------------------------------------|----------------------------------------------------------------|---------------------------------------------------------------------------------|
| Hexanimidoyl                                         | $\text{CH}_3\text{—}[\text{CH}_2]_4\text{—C(=NH)—}$                     | Iodonio                                                        | $^+\text{HI—}$                                                                  |
| Hexanoyl                                             | $\text{CH}_3\text{—}[\text{CH}_2]_4\text{—CO—}$                         | Iodosyl                                                        | $\text{OI—}$                                                                    |
| Hexanoylamino                                        | $\text{CH}_3\text{—}[\text{CH}_2]_4\text{—CO—NH—}$                      | Iodyl                                                          | $\text{O}_2\text{I—}$                                                           |
| Hexyl                                                | $\text{CH}_3\text{—}[\text{CH}_2]_4\text{—CH}_2\text{—}$                | Isobutoxy ( <i>unsubstituted only</i> )                        | $(\text{CH}_3)_2\text{CH—CH}_2\text{—O—}$                                       |
| Hexylidene                                           | $\text{CH}_3\text{—}[\text{CH}_2]_4\text{—CH=}$                         | Isobutyl ( <i>unsubstituted only</i> )                         | $(\text{CH}_3)_2\text{CH—CH}_2\text{—}$                                         |
| Hexyloxy                                             | $\text{CH}_3[\text{CH}_2]_5\text{—O—}$                                  | Isobutylidene ( <i>unsubstituted only</i> )                    | $(\text{CH}_3)_2\text{CH—CH=}$                                                  |
| Hippuryl                                             | $\text{C}_6\text{H}_5\text{—CO—NH—CH}_2\text{—CO—}$                     | Isobutylidyne ( <i>unsubstituted only</i> )                    | $(\text{CH}_3)_2\text{CH—C}\equiv$                                              |
| Histidyl                                             | $\text{N}_2\text{C}_3\text{H}_3\text{—CH}_2\text{—CH(NH}_2\text{)—CO—}$ | Isobutyryl ( <i>unsubstituted only; or 2-methylpropanoyl</i> ) | $(\text{CH}_3)_2\text{CH—CO—}$                                                  |
| Homocysteinyl                                        | $\text{HS—CH}_2\text{—CH}_2\text{—CH(NH}_2\text{)—CO—}$                 | Isocarbonohydrazido                                            | $\text{H}_2\text{N—N=C(OH)—NH—NH—}$                                             |
| Homoseryl                                            | $\text{HO—CH}_2\text{—CH}_2\text{—CH(NH}_2\text{)—CO—}$                 | Isocrotonoyl                                                   | $\text{CH}_3\text{—CH=CH—CO— (cis)}$                                            |
| Hydantoyl                                            | $\text{H}_2\text{N—CO—NH—CH}_2\text{—CO—}$                              | Isocyanato                                                     | $\text{OCN—}$                                                                   |
| Hydratropoyl ( <i>or 2-phenylpropanoyl</i> )         | $\text{C}_6\text{H}_5\text{—CH(CH}_3\text{)—CO—}$                       | Isocyano                                                       | $\text{CN—}$                                                                    |
| Hydrazi                                              | $\text{—NH—NH— (to single atom)}$                                       | Isohexyl ( <i>unsubstituted only</i> )                         | $(\text{CH}_3)_2\text{CH—}[\text{CH}_2]_3\text{—}$                              |
| Hydrazino                                            | $\text{H}_2\text{N—NH—}$                                                | Isoleucyl                                                      | $\text{C}_2\text{H}_5\text{—CH(CH}_3\text{)—CH(NH}_2\text{)—CO}$                |
| Hydrazo                                              | $\text{—NH—NH— (to different atoms)}$                                   | Isonicotinoyl ( <i>or 4-pyridinecarbonyl</i> )                 | $\text{NC}_5\text{H}_4\text{—CO— (4-)}$                                         |
| Hydrazono                                            | $\text{H}_2\text{N—N=}$                                                 | Isopentyl ( <i>unsubstituted only</i> )                        | $(\text{CH}_3)_2\text{CH—CH}_2\text{—CH}_2\text{—}$                             |
| Hydroperoxy                                          | $\text{HO—O—}$                                                          | Isophthaloyl ( <i>or 1,3-benzenedicarbonyl</i> )               | $\text{—CO—C}_6\text{H}_4\text{—CO— (m-)}$                                      |
| Hydroseleno                                          | $\text{HSe—}$                                                           | Isopropenyl ( <i>unsubstituted only; or 1-methylvinyl</i> )    | $\text{CH}_2=\text{C(CH}_3\text{)—}$                                            |
| Hydroxy                                              | $\text{HO—}$                                                            | Isopropoxy ( <i>unsubstituted only</i> )                       | $(\text{CH}_3)_2\text{CH—O—}$                                                   |
| Hydroxyamino                                         | $\text{HO—NH—}$                                                         | Isopropyl ( <i>unsubstituted only</i> )                        | $(\text{CH}_3)_2\text{CH—}$                                                     |
| <i>o</i> -Hydroxybenzoyl ( <i>or salicyloyl</i> )    | $\text{o-HO—C}_6\text{H}_4\text{—CO—}$                                  | <i>p</i> -Isopropylbenzoyl                                     | $\textit{p}\text{-(CH}_3)_2\text{CH—C}_6\text{H}_4\text{—CO—}$                  |
| <i>m</i> -Hydroxybenzoyl                             | $\textit{m}\text{-HO—C}_6\text{H}_4\text{—CO—}$                         | Isopropylbenzyl                                                | $(\text{CH}_3)_2\text{CH—C}_6\text{H}_4\text{—CH}_2\text{—}$                    |
| <i>p</i> -Hydroxybenzoyl                             | $\textit{p}\text{-HO—C}_6\text{H}_4\text{—CO—}$                         | Isopropylidene                                                 | $(\text{CH}_3)_2\text{C=}$                                                      |
| Hydroxybutanedioyl, <i>see</i> Maloyl                |                                                                         | Isoselenocyanato                                               | $\text{SeCN—}$                                                                  |
| 2-Hydroxy-2,2-diphenylethanoyl, <i>see</i> Benziloyl |                                                                         | Isosemicarbazido                                               | $\text{H}_2\text{N—NH—C(OH)=N—}$                                                |
| Hydroxyethanoyl, <i>see</i> Glycoloyl                |                                                                         | Isothiocyanato                                                 | $\text{SCN—}$                                                                   |
| Hydroxyimino                                         | $\text{HO—N=}$                                                          | Isothioureido                                                  | $\text{HN=C(SH)—NH—, H}_2\text{N—C(SH)=N—, HN=C(OH)—NH—, H}_2\text{N—C(OH)=N—}$ |
| 4-Hydroxy-3-methoxybenzoyl ( <i>or vanilloyl</i> )   | $\text{4-HO, 3-CH}_3\text{O—C}_6\text{H}_3\text{—CO—}$                  | Isoureido                                                      | $(\text{CH}_3)_2\text{CH—CH}_2\text{—CO—}$                                      |
| 3-Hydroxy-2-phenylpropanoyl ( <i>or tropoyl</i> )    | $\text{C}_6\text{H}_5\text{—CH(CH}_2\text{OH)—CO—}$                     | Isovaleryl ( <i>unsubstituted only; or 3-methylbutanoyl</i> )  |                                                                                 |
| Hydroxypropanedioyl ( <i>or tartronoyl</i> )         | $\text{—CO—CH(OH)—CO—}$                                                 | Lactoyl                                                        | $\text{CH}_3\text{—CH(OH)—CO—}$                                                 |
| 2-Hydroxypropanoyl ( <i>or lactoyl</i> )             | $\text{CH}_3\text{—CH(OH)—CO—}$                                         | Lauroyl ( <i>unsubstituted only</i> )                          | $\text{CH}_3\text{—}[\text{CH}_2]_{10}\text{—CO—}$                              |
| Icosyl                                               | $\text{CH}_3\text{—}[\text{CH}_2]_{18}\text{—CH}_2\text{—}$             |                                                                |                                                                                 |
| Imino                                                | $\text{—NH—, HN=}$                                                      |                                                                |                                                                                 |
| Iminomethylamino                                     | $\text{HN=CH—NH—}$                                                      |                                                                |                                                                                 |
| Iodo                                                 | $\text{I—}$                                                             |                                                                |                                                                                 |
| Iodoformyl                                           | $\text{I—CO—}$                                                          |                                                                |                                                                                 |

**TABLE 1.13** Names and Formulas of Organic Radicals (*Continued*)

| Name                                                    | Formula                                                                                | Name                                      | Formula                                                                           |
|---------------------------------------------------------|----------------------------------------------------------------------------------------|-------------------------------------------|-----------------------------------------------------------------------------------|
| Leucyl                                                  | $(\text{CH}_3)_2\text{CH}-\text{CH}_2-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$         | 5-Methylhexyl                             | $(\text{CH}_3)_2\text{CH}-[\text{CH}_2]_4-$                                       |
| Lysyl                                                   | $\text{H}_2\text{N}-[\text{CH}_2]_4-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$           | Methylidyne                               | $\text{HC}\equiv$                                                                 |
| Maleoyl                                                 | $-\text{CO}-\text{CH}=\text{CH}-\text{CO}-$                                            | Methylsulfinimidoyl                       | $\text{CH}_3-\text{S}(=\text{NH})-$                                               |
| Malonyl                                                 | $-\text{CO}-\text{CH}_2-\text{CO}-$                                                    | Methylsulfinohydrazonoyl                  | $\text{CH}_3-\text{S}(=\text{NNH}_2)-$                                            |
| Maloyl                                                  | $-\text{CO}-\text{CH}(\text{OH})-\text{CH}_2-$<br>$\text{CO}-$                         | Methylsulfinohydroxi-<br>moyl             | $\text{CH}_3-\text{S}(=\text{N}-\text{OH})-$                                      |
| Mercapto-                                               | $\text{HS}-$                                                                           | Methylsulfinyl                            | $\text{CH}_3-\text{SO}-$                                                          |
| Mesaconoyl ( <i>unsubstituted only</i> )                | $-\text{CO}-\text{CH}=\text{CH}-\text{CO}-$<br>$\text{CH}_3-\text{C}-\text{CO}-$       | Methylsulfinylamino                       | $\text{CH}_3-\text{SO}-\text{NH}-$                                                |
| Mesityl                                                 | $2,4,6-(\text{CH}_3)_3\text{C}_6\text{H}_2-$                                           | Methylsulfonyldiazo-<br>nonyl             | $\text{CH}_3-\text{S}(\text{O})(\text{NNH}_2)-$                                   |
| Mesoxalo                                                | $\text{HOOC}-\text{CO}-\text{CO}-$                                                     | Methylsulfonylimidoyl                     | $\text{CH}_3-\text{S}(\text{O})(=\text{NH})-$                                     |
| Mesoxalyl                                               | $-\text{CO}-\text{CO}-\text{CO}-$                                                      | Methylsulfonylhydroxa-<br>moyl            | $\text{CH}_3-\text{S}(\text{O})(\text{N}-\text{OH})-$                             |
| Mesyl                                                   | $\text{CH}_3-\text{SO}_2-$                                                             | Methylsulfonyl                            | $\text{CH}_3-\text{SO}_2-$                                                        |
| Methacryloyl ( <i>or 2-methyl-propenoyl</i> )           | $\text{CH}_2=\text{C}(\text{CH}_3)-\text{CO}-$                                         | Methylthio                                | $\text{CH}_3\text{S}-$                                                            |
| Methaneazo                                              | $\text{CH}_3-\text{N}=\text{N}-$                                                       | (Methylthio)sulfonyl                      | $\text{CH}_3\text{S}-\text{SO}_2-$                                                |
| Methaneazoxy                                            | $\text{CH}_3-\text{N}_2\text{O}-$                                                      | 1-Methylvinyl, <i>see</i> Isopropenyl     |                                                                                   |
| Methanesulfinamido                                      | $\text{CH}_3-\text{SO}-\text{NH}-$                                                     | Morpholino (4- <i>only</i> )              |  |
| Methanesulfinyl                                         | $\text{CH}_3-\text{SO}-$                                                               | Morpholinyl (3- <i>shown</i> )            |  |
| Methanesulfonamido                                      | $\text{CH}_3-\text{SO}_2-\text{NH}-$                                                   | Myristoyl ( <i>unsubstituted only</i> )   | $\text{CH}_3-[\text{CH}_2]_{12}-\text{CO}-$                                       |
| Methanesulfonyl, <i>see</i> Mesyl                       |                                                                                        | Naphthalenazo                             | $\text{C}_{10}\text{H}_7-\text{N}=\text{N}-$                                      |
| Methanoyl, <i>see</i> Formyl                            |                                                                                        | Naphthalenecarbonyl, <i>see</i> Naphthoyl |                                                                                   |
| Methionyl                                               | $\text{CH}_3-\text{S}-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$ | Naphthoyl                                 | $\text{C}_{10}\text{H}_7-\text{CO}-$                                              |
| Methoxalyl                                              | $\text{CH}_3\text{OOC}-\text{CO}-$                                                     | Naphthoyloxy                              | $\text{C}_{10}\text{H}_7-\text{CO}-\text{O}-$                                     |
| Methoxy                                                 | $\text{CH}_3\text{O}-$                                                                 | Naphthyl                                  | $\text{C}_{10}\text{H}_7-$                                                        |
| Methoxybenzoyl ( <i>o</i> -, <i>m</i> -, <i>or p</i> -) | $\text{CH}_3\text{O}-\text{C}_6\text{H}_4-\text{CO}-$                                  | Naphthylazo                               | $\text{C}_{10}\text{H}_7-\text{N}=\text{N}-$                                      |
| Methoxycarbonyl                                         | $\text{CH}_3\text{O}-\text{CO}-$                                                       | Naphthylene                               | $-\text{C}_{10}\text{H}_6-$                                                       |
| Methoxyimino                                            | $\text{CH}_3\text{O}-\text{N}=\text{N}-$                                               | Naphthylenebisazo                         | $-\text{N}=\text{N}-\text{C}_{10}\text{H}_6-$                                     |
| Methoxyphenyl                                           | $\text{CH}_3\text{O}-\text{C}_6\text{H}_4-$                                            |                                           | $\text{N}=\text{N}-$                                                              |
| Methoxysulfinyl                                         | $\text{CH}_3\text{O}-\text{SO}-$                                                       | Naphthylloxy                              | $\text{C}_{10}\text{H}_7-\text{O}-$                                               |
| Methoxysulfonyl                                         | $\text{CH}_3\text{O}-\text{SO}_2-$                                                     | Neopentyl ( <i>unsubstituted only</i> )   | $(\text{CH}_3)_3\text{C}-\text{CH}_2-$                                            |
| Methoxy(thiosulfonyl)                                   | $\text{CH}_3\text{O}-\text{S}_2\text{O}-$                                              | Nicotinoyl                                | $\text{NC}_5\text{H}_4-\text{CO}-$ (3-)                                           |
| Methyl                                                  | $\text{CH}_3-$                                                                         | Nitrilo                                   | $\text{N}\equiv$                                                                  |
| Methylallyl                                             | $\text{CH}_2=\text{C}(\text{CH}_3)-\text{CH}_2-$                                       | Nitro                                     | $\text{O}_2\text{N}-$                                                             |
| Methylamino                                             | $\text{CH}_3-\text{NH}-$                                                               | <i>aci</i> -Nitro                         | $\text{HO}-(\text{O}=\text{N})=$                                                  |
| Methylazo                                               | $\text{CH}_3-\text{N}=\text{N}-$                                                       | Nitroso                                   | $\text{ON}-$                                                                      |
| Methylazoxy                                             | $\text{CH}_3-\text{N}_2\text{O}-$                                                      | Nonanedioyl                               | $-\text{CO}-[\text{CH}_2]_7-\text{CO}-$                                           |
| $\alpha$ -Methylbenzyl                                  | $\text{C}_6\text{H}_5-\text{CH}(\text{CH}_3)-$                                         | Nonanoyl                                  | $\text{CH}_3-[\text{CH}_2]_7-\text{CO}-$                                          |
| Methylbenzyl                                            | $\text{CH}_3-\text{C}_6\text{H}_4-\text{CH}_2-$                                        | Nonyl                                     | $\text{CH}_3-[\text{CH}_2]_7-\text{CH}_2-$                                        |
| 3-Methylbutanoyl                                        | $(\text{CH}_3)_2\text{CH}-\text{CH}_2-\text{CO}-$                                      | Norbornyl                                 | $\text{C}_7\text{H}_{11}-$                                                        |
| <i>cis</i> -Methylbutenedioyl                           | $\text{HC}=\text{CO}-$<br>$\text{CH}_3-\text{C}-\text{CO}-$                            | Norbornyl, <i>see</i> Norbornyl           |                                                                                   |
| <i>trans</i> -Methylbutenedioyl                         | $-\text{CO}-\text{CH}=\text{CH}-\text{CO}-$<br>$\text{CH}_3-\text{C}-\text{CO}-$       | Norcamphyl, <i>see</i> Norbornyl          |                                                                                   |
| Methyldithio                                            | $\text{CH}_3-\text{S}-\text{S}-$                                                       | Norleucyl                                 | $\text{CH}_3-[\text{CH}_2]_3-\text{CH}(\text{NH}_2)-\text{CO}-$                   |
| Methylene                                               | $-\text{CH}_2-$ , $\text{H}_2\text{C}=\text{CH}_2$                                     | Norvalyl                                  | $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}(\text{NH}_2)-\text{CO}-$           |
| Methylenedioxy                                          | $-\text{O}-\text{CH}_2-\text{O}-$                                                      | Octadecanoyl                              | $\text{CH}_3-[\text{CH}_2]_{16}-\text{CO}-$                                       |
| 3,4-Methylenedioxybenzoyl                               | $3,4-\text{CH}_2\text{O}_2:\text{C}_6\text{H}_3-\text{CO}-$                            |                                           |                                                                                   |

**TABLE 1.13** Names and Formulas of Organic Radicals (*Continued*)

| Name                                                 | Formula                                                                        | Name                                             | Formula                                                                                                                                                                    |
|------------------------------------------------------|--------------------------------------------------------------------------------|--------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>cis</i> -9-Octadecenoyl                           | $\text{H}[\text{CH}_2]_8-\text{CH}=\text{CH}-$<br>$[\text{CH}_2]_7-\text{CO}-$ | Phenylsulfamoyl                                  | $\text{C}_6\text{H}_5-\text{NH}-\text{SO}_2$                                                                                                                               |
| Octadecyl                                            | $\text{CH}_3-[\text{CH}_2]_{16}-\text{CH}_2-$                                  | Phenylsulfinyl                                   | $\text{C}_6\text{H}_5-\text{SO}-$                                                                                                                                          |
| Octanediol                                           | $-\text{CO}-[\text{CH}_2]_6-\text{CO}-$                                        | Phenylsulfonyl                                   | $\text{C}_6\text{H}_5-\text{SO}_2-$                                                                                                                                        |
| Octanoyl                                             | $\text{CH}_3-[\text{CH}_2]_6-\text{CO}-$                                       | Phenylsulfonylamino                              | $\text{C}_6\text{H}_5-\text{SO}_2-\text{NH}-$                                                                                                                              |
| Octyl                                                | $\text{CH}_3-[\text{CH}_2]_6-\text{CH}_2-$                                     | Phenylthio                                       | $\text{C}_6\text{H}_5-\text{S}-$                                                                                                                                           |
| Oleoyl                                               | $\text{H}[\text{CH}_2]_8-\text{CH}=\text{CH}-$<br>$[\text{CH}_2]_7-\text{CO}-$ | 3-Phenylureido                                   | $\text{C}_6\text{H}_5-\text{NH}-\text{CO}-\text{NH}-$                                                                                                                      |
| Ornithyl                                             | $\text{H}_2\text{N}-[\text{CH}_2]_3-$<br>$\text{CH}(\text{NH}_2)-\text{CO}-$   | Phthalamoyl                                      | $\text{H}_2\text{N}-\text{CO}-\text{C}_6\text{H}_4-\text{CO}-$<br>( <i>o</i> -)                                                                                            |
| Oxalacetyl                                           | $-\text{CO}-\text{CH}_2-\text{CO}-$<br>$\text{CO}-$                            | Phthalidyl                                       | $\text{C}_6\text{H}_4-\text{CO}-\text{O}-\text{CH}-$<br>$\text{CO}-\text{C}_6\text{H}_4-\text{CO}-\text{N}-$<br>$-\text{CO}-\text{C}_6\text{H}_4-\text{CO}-$ ( <i>o</i> -) |
| Oxalaceto                                            | $\text{HOOC}-\text{CO}-\text{CH}_2-$<br>$\text{CO}-$                           | Picryl                                           | $2,4,6-(\text{NO}_2)_3\text{C}_6\text{H}_2-$                                                                                                                               |
| Oxalo                                                | $\text{HOOC}-\text{CO}-$                                                       | Pimeloyl ( <i>unsubstituted</i><br><i>only</i> ) | $-\text{CO}-[\text{CH}_2]_5-\text{CO}-$                                                                                                                                    |
| Oxalyl                                               | $-\text{CO}-\text{CO}-$                                                        | Piperidino ( <i>1- only</i> )                    | $\text{C}_5\text{H}_{10}\text{N}-$                                                                                                                                         |
| Oxamoyl                                              | $\text{H}_2\text{N}-\text{CO}-\text{CO}-$                                      | Piperidyl (2-, 3-, 4-)                           | $\text{NC}_5\text{H}_{10}-$                                                                                                                                                |
| Oxido                                                | $^-\text{O}-$ (ion)                                                            | Piperonyl                                        | $3,4-\text{CH}_2\text{O}_2:\text{C}_6\text{H}_3-\text{CH}_2-$                                                                                                              |
| Oxo                                                  | $\text{O}=\text{O}$                                                            | Pivaloyl ( <i>unsubstituted</i><br><i>only</i> ) | $(\text{CH}_3)_3\text{C}-\text{CO}-$                                                                                                                                       |
| Oxonio                                               | $^+\text{H}_3\text{O}-$                                                        | Polythio                                         | $-\text{S}_4-$                                                                                                                                                             |
| Oxy                                                  | $-\text{O}-$                                                                   | Propanedioyl, <i>see</i> Ma-<br>lonyl            |                                                                                                                                                                            |
| Palmitoyl ( <i>unsubstituted</i><br><i>only</i> )    | $\text{CH}_3-[\text{CH}_2]_{14}-\text{CO}-$                                    | Propanoyl, <i>see</i> Propionyl                  |                                                                                                                                                                            |
| Pentafluorothio                                      | $\text{F}_5\text{S}-$                                                          | Propargyl, <i>see</i> 2-Pro-<br>pynyl            |                                                                                                                                                                            |
| Pentamethylene                                       | $-\text{CH}_2-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}_2-\text{CH}_2-$          | Propenoyl, <i>see</i> Acryloyl                   |                                                                                                                                                                            |
| Pentanedioyl, <i>see</i> Glu-<br>taryl               |                                                                                | 1-Propenyl                                       | $\text{CH}_3-\text{CH}=\text{CH}-$                                                                                                                                         |
| Pentanoyl, <i>see</i> Valeryl                        |                                                                                | 2-Propenyl, <i>see</i> Allyl                     |                                                                                                                                                                            |
| Pentenyl (2- <i>shown</i> )                          | $\text{CH}_3-\text{CH}_2-\text{CH}=\text{CH}-$<br>$\text{CH}_2-$               | Propenylene                                      | $-\text{CH}_2-\text{CH}=\text{CH}-$                                                                                                                                        |
| Pentyl                                               | $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}_2-$           | Propioloyl                                       | $\text{CH}\equiv\text{C}-\text{CO}-$                                                                                                                                       |
| Pentyloxy                                            | $\text{CH}_3-[\text{CH}_2]_4-\text{O}-$                                        | Propionamido                                     | $\text{CH}_3-\text{CH}_2-\text{CO}-\text{NH}-$                                                                                                                             |
| Perchloryl                                           | $\text{O}_3\text{Cl}-$                                                         | Propionyl                                        | $\text{CH}_3-\text{CH}_2-\text{CO}-$                                                                                                                                       |
| Phenacyl                                             | $\text{C}_6\text{H}_5-\text{CO}-\text{CH}_2-$                                  | Propionylamino                                   | $\text{CH}_3-\text{CH}_2-\text{CO}-\text{NH}-$                                                                                                                             |
| Phenacylidene                                        | $\text{C}_6\text{H}_5-\text{CO}-\text{CH}=\text{CH}_2-$                        | Propionyloxy                                     | $\text{CH}_3-\text{CH}_2-\text{CO}-\text{O}-$                                                                                                                              |
| Phenanthryl                                          | $\text{C}_{14}\text{H}_9-$                                                     | Propoxy                                          | $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{O}-$                                                                                                                            |
| Phenethyl                                            | $\text{C}_6\text{H}_5-\text{CH}_2-\text{CH}_2-$                                | Propyl                                           | $\text{CH}_3-\text{CH}_2-\text{CH}_2-$                                                                                                                                     |
| Phenetidino ( <i>o</i> -, <i>m</i> -, or <i>p</i> -) | $\text{C}_6\text{H}_5\text{O}-\text{C}_6\text{H}_4-\text{NH}-$                 | Propylene                                        | $-\text{CH}(\text{CH}_3)-\text{CH}_2-$                                                                                                                                     |
| Phenoxy                                              | $\text{C}_6\text{H}_5-\text{O}-$                                               | Propylidene                                      | $\text{CH}_3-\text{CH}_2-\text{CH}=\text{CH}_2-$                                                                                                                           |
| Phenyl                                               | $\text{C}_6\text{H}_5-$                                                        | Propylidyne                                      | $\text{CH}_3-\text{CH}_2-\text{C}\equiv\text{C}-$                                                                                                                          |
| Phenylacetyl                                         | $\text{C}_6\text{H}_5-\text{CH}_2-\text{CO}-$                                  | Propynoyl, <i>see</i> Propiolyl                  |                                                                                                                                                                            |
| Phenylazo                                            | $\text{C}_6\text{H}_5-\text{N}=\text{N}-$                                      | 1-Propynyl                                       | $\text{CH}_3-\text{C}\equiv\text{C}-$                                                                                                                                      |
| Phenylazoxy                                          | $\text{C}_6\text{H}_5-\text{N}_2\text{O}-$                                     | 2-Propynyl                                       | $\text{HC}\equiv\text{C}-\text{CH}_2-$                                                                                                                                     |
| Phenylcarbamoyl                                      | $\text{C}_6\text{H}_5-\text{NH}-\text{CO}-$<br>$-\text{C}_6\text{H}_4-$        | Protocatechuoyl                                  | $3,4-(\text{HO})_2\text{C}_6\text{H}_3-\text{CO}-$                                                                                                                         |
| Phenylene                                            | $-\text{N}=\text{N}-\text{C}_6\text{H}_4-$                                     | 3-Pyridinecarbonyl                               | $\text{NC}_5\text{H}_4-\text{CO}-$ (3-)                                                                                                                                    |
| Phenylenebisazo                                      | $\text{N}=\text{N}-$                                                           | 4-Pyridinecarbonyl                               | $\text{NC}_5\text{H}_4-\text{CO}-$ (4-)                                                                                                                                    |
| Phenylimino                                          | $\text{C}_6\text{H}_5-\text{N}=\text{N}-$                                      | Pyridinio                                        | $^+\text{NC}_5\text{H}_5-$ (ion)                                                                                                                                           |
| 2-Phenylpropanoyl                                    | $\text{C}_6\text{H}_5-\text{CH}(\text{CH}_3)-\text{CO}-$                       | Pyridyl                                          | $\text{NC}_5\text{H}_4-$                                                                                                                                                   |
| 3-Phenylpropanoyl, <i>see</i><br>Cinnamoyl           |                                                                                | 2-Pyridylcarbonyl                                | $\text{NC}_5\text{H}_4-\text{CO}-$ (2-)                                                                                                                                    |
| 3-Phenylpropyl                                       | $\text{C}_6\text{H}_5-\text{CH}_2-\text{CH}_2-$<br>$\text{CH}_2-$              | Pyridyloxy                                       | $\text{NC}_5\text{H}_4-\text{O}-$                                                                                                                                          |
|                                                      |                                                                                | Pyruvoyl                                         | $\text{CH}_3-\text{CO}-\text{CO}-$                                                                                                                                         |
|                                                      |                                                                                | Salicyl                                          | $o\text{-HO}-\text{C}_6\text{H}_4-\text{CH}_2-$                                                                                                                            |
|                                                      |                                                                                | Salicylidene                                     | $o\text{-HO}-\text{C}_6\text{H}_4-\text{CH}=\text{CH}_2-$                                                                                                                  |
|                                                      |                                                                                | Salicyloyl                                       | $o\text{-HO}-\text{C}_6\text{H}_4-\text{CO}-$                                                                                                                              |
|                                                      |                                                                                | Sarcosyl                                         | $\text{CH}_3-\text{NH}-\text{CH}_2-\text{CO}-$                                                                                                                             |

**TABLE 1.13** Names and Formulas of Organic Radicals (*Continued*)

| Name                                   | Formula                                                                                                                                        | Name                                               | Formula                                                                                                                                   |
|----------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Sebacoyl ( <i>unsubstituted only</i> ) | $-\text{CO}-[\text{CH}_2]_8-\text{CO}-$                                                                                                        | (Terthiophenyl)                                    | $\text{SC}_4\text{H}_3-\text{SC}_4\text{H}_2-\text{SC}_4\text{H}_2-$                                                                      |
| Seleneno                               | $\text{HOSe}-$                                                                                                                                 | Tetradecanoyl                                      | $\text{CH}_3-[\text{CH}_2]_{12}-\text{CO}-$                                                                                               |
| Selenino                               | $\text{HO}_2\text{Se}-$                                                                                                                        | Tetradecyl                                         | $\text{CH}_3-[\text{CH}_2]_{12}-\text{CH}_2-$                                                                                             |
| Seleninyl                              | $\text{OSe}=\text{}$                                                                                                                           | Tetramethylene                                     | $-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-$                                                                                       |
| Seleno                                 | $-\text{Se}-$                                                                                                                                  |                                                    |                                                                                                                                           |
| Selenocyanato                          | $\text{NC}-\text{Se}-$                                                                                                                         | Thenoyl (2- shown)                                 | $\begin{array}{c} \text{CH}=\text{C}-\text{CO}- \\   \quad \quad \quad \diagdown \\ \text{CH}=\text{CH} \quad \quad \text{S} \end{array}$ |
| Selenoformyl                           | $\text{HSeC}-$                                                                                                                                 | Thenyl                                             | $\text{SC}_4\text{H}_3-\text{CH}_2-$                                                                                                      |
| Selenonio                              | $^+\text{H}_2\text{Se}-$ (ion)                                                                                                                 | Thienyl                                            | $\text{SC}_4\text{H}_3-$                                                                                                                  |
| Selenono                               | $\text{HO}_3\text{Se}-$                                                                                                                        | Thio                                               | $-\text{S}-$                                                                                                                              |
| Selenonyl                              | $\text{O}_2\text{Se}-$                                                                                                                         | Thioacetyl                                         | $\text{CH}_3-\text{CS}-$                                                                                                                  |
| Selenoureido                           | $\text{H}_2\text{N}-\text{CSe}-\text{NH}-$                                                                                                     | Thiobenzoyl                                        | $\text{C}_6\text{H}_5-\text{CS}-$                                                                                                         |
| Selenoxo                               | $(\text{C})=\text{Se}$                                                                                                                         | Thiocarbamoyl                                      | $\text{H}_2\text{N}-\text{CS}-$                                                                                                           |
| Semicarbazido                          | $\text{H}_2\text{N}-\text{CO}-\text{NH}-\text{NH}-$                                                                                            | Thiocarbazono                                      | $\text{HN}=\text{N}-\text{CS}-\text{NH}-$                                                                                                 |
| Semicarbazono                          | $\text{H}_2\text{N}-\text{CO}-\text{NH}-\text{N}=\text{}$                                                                                      |                                                    | $\text{NH}-$                                                                                                                              |
| Seryl                                  | $\text{HO}-\text{CH}_2-\text{CH}(\text{NH}_2)-\text{CO}-$                                                                                      | Thiocarbodiazono                                   | $\text{HN}=\text{N}-\text{CS}-\text{N}=\text{N}-$                                                                                         |
|                                        | $\text{CO}-$                                                                                                                                   | Thiocarbonohydrazido                               | $\text{H}_2\text{N}-\text{NH}-\text{CS}-\text{NH}-$                                                                                       |
| Stearoyl ( <i>unsubstituted only</i> ) | $\text{CH}_3-[\text{CH}_2]_{16}-\text{CO}-$                                                                                                    |                                                    | $\text{NH}-$                                                                                                                              |
| Styryl                                 | $\text{C}_6\text{H}_5-\text{CH}=\text{CH}-$                                                                                                    | Thiocarbonyl                                       | $-\text{CS}-, \text{SC}=\text{}$                                                                                                          |
| Suberoyl ( <i>unsubstituted only</i> ) | $-\text{CO}-[\text{CH}_2]_6-\text{CO}-$                                                                                                        | Thiocarboxy                                        | $\text{HSOC}-, \text{HS}-\text{CO}-$                                                                                                      |
| Succinamoyl                            | $\text{H}_2\text{N}-\text{CO}-\text{CH}_2-\text{CH}_2-\text{CO}-$                                                                              | Thiocyanato                                        | $\text{NCS}-$                                                                                                                             |
|                                        | $\text{CO}-$                                                                                                                                   | Thioformyl                                         | $\text{SHC}-, \text{HCS}-$                                                                                                                |
|                                        | $\begin{array}{c} \text{CH}_2-\text{C}=\text{O} \\   \quad \quad \diagdown \\ \text{CH}_2-\text{C}=\text{O} \quad \quad \text{N}- \end{array}$ | Thiophenecarbonyl, <i>see</i> Thenoyl              |                                                                                                                                           |
| Succinimido                            |                                                                                                                                                | Thiosemicarbazido                                  | $\text{H}_2\text{N}-\text{CS}-\text{NH}-\text{NH}-$                                                                                       |
|                                        |                                                                                                                                                | Thiosulfinio                                       | $\text{HOS}_2-$                                                                                                                           |
| Succinimidoyl                          | $-\text{C}(=\text{NH})-\text{CH}_2-\text{CH}_2\text{C}(=\text{NH})-$                                                                           | Thiosulfo                                          | $\text{HO}_2\text{S}_2-$                                                                                                                  |
|                                        | $-\text{CO}-\text{CH}_2-\text{CH}_2-\text{CO}-$                                                                                                | Thioreido                                          | $\text{H}_2\text{N}-\text{CS}-\text{NH}-$                                                                                                 |
| Succinyl                               | $\text{H}_2\text{N}-\text{SO}_2-$                                                                                                              | Thioxo                                             | $\text{S}=\text{}$                                                                                                                        |
| Sulfamoyl                              | $p\text{-H}_2\text{N}-\text{C}_6\text{H}_4-\text{SO}_2-\text{NH}-$                                                                             | Threonyl                                           | $\text{CH}_3-\text{CH}(\text{OH})-\text{CH}(\text{NH}_2)-\text{CO}-$                                                                      |
| Sulfanilamido                          | $p\text{-H}_2\text{N}-\text{C}_6\text{H}_4-\text{SO}_2-$                                                                                       | Toluenesulfonyl ( <i>o</i> -, <i>m</i> -)          | $\text{CH}_3-\text{C}_6\text{H}_4-\text{SO}_2-$                                                                                           |
|                                        | $\text{H}_2\text{N}-\text{S}-$                                                                                                                 | Toluidino ( <i>o</i> -, <i>m</i> -, or <i>p</i> -) | $\text{CH}_3-\text{C}_6\text{H}_4-\text{NH}-$                                                                                             |
| Sulfanilyl                             | $\text{HO}-\text{S}-$                                                                                                                          | Toluyol ( <i>o</i> -, <i>m</i> -, or <i>p</i> -)   | $\text{CH}_3-\text{C}_6\text{H}_4-\text{CO}-$                                                                                             |
| Sulfenamoyl                            | $-\text{S}-$ (ion)                                                                                                                             | Tolylsulfonyl                                      | $\text{CH}_3-\text{C}_6\text{H}_4-$                                                                                                       |
| Sulfeno                                | $\text{H}_2\text{N}-\text{SO}-$                                                                                                                | Tosyl ( <i>p</i> - only)                           | $\text{CH}_3-\text{C}_6\text{H}_4-\text{SO}_2-$                                                                                           |
| Sulfido                                | $\text{HO}_2\text{S}-$                                                                                                                         | Triazano                                           | $p\text{-CH}_3-\text{C}_6\text{H}_4-\text{SO}_2-$                                                                                         |
| Sulfinamoyl                            | $-\text{SO}-$                                                                                                                                  | Triazeno                                           | $\text{H}_2\text{N}-\text{NH}-\text{NH}-$                                                                                                 |
| Sulfino                                | $\text{HO}-\text{SO}_2-$                                                                                                                       | Trichlorothio                                      | $\text{H}_2\text{N}-\text{N}=\text{N}-$                                                                                                   |
| Sulfinyl                               | $\text{CH}(\text{OH})-\text{CO}-$                                                                                                              | Tridecanoyl                                        | $\text{Cl}_3\text{S}-$                                                                                                                    |
| Sulfo                                  | $-\text{CO}-\text{CH}(\text{OH})-\text{CO}-$                                                                                                   | Tridecyl                                           | $\text{CH}_3-[\text{CH}_2]_{11}-\text{CO}-$                                                                                               |
| Sulfoamino                             | $\text{HO}_2\text{S}-\text{NH}-$                                                                                                               | Trifluorothio                                      | $\text{CH}_3-[\text{CH}_2]_{12}-$                                                                                                         |
| Sulfonato                              | $-\text{O}_3\text{S}-$ (ion)                                                                                                                   | 3,4,5-Trihydroxybenzoyl                            | $\text{F}_3\text{S}-$                                                                                                                     |
| Sulfonio                               | $^+\text{H}_2\text{S}-$ (ion)                                                                                                                  | Trimethylammonio                                   | $3,4,5\text{-(HO)}_3\text{C}_6\text{H}_2-\text{CO}-$                                                                                      |
| Sulfonyl                               | $-\text{SO}_2-$                                                                                                                                | Trimethylanilino ( <i>all isomers</i> )            | $(\text{CH}_3)_3\text{N}^+-$ (ion)                                                                                                        |
| Sulfonyldioxy                          | $-\text{O}-\text{SO}_2-\text{O}-$                                                                                                              | Trimethylene                                       | $(\text{CH}_3)_3\text{C}_6\text{H}_2-\text{NH}-$                                                                                          |
| Tartaroyl                              | $\text{CH}(\text{OH})-\text{CO}-$                                                                                                              | Trimethylenedioxy                                  | $-\text{CH}_2-\text{CH}_2-\text{CH}_2-$                                                                                                   |
|                                        | $-\text{CO}-\text{CH}(\text{OH})-\text{CO}-$                                                                                                   |                                                    | $-\text{O}-\text{CH}_2-\text{CH}_2-$                                                                                                      |
| Tartronyl                              | $\text{H}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{SO}_2-$                                                                                      |                                                    | $\text{CH}_2-\text{O}-$                                                                                                                   |
| Tauryl                                 | $\text{Te}$ replacing $\text{O}$                                                                                                               | Triphenylmethyl                                    | $(\text{C}_6\text{H}_5)_3\text{C}-$                                                                                                       |
| Telluro                                | $-\text{CO}-\text{C}_6\text{H}_4-\text{CO}-$ ( <i>p</i> -)                                                                                     | Trithio                                            | $-\text{S}_3-$                                                                                                                            |
| Terephthaloyl                          | $\text{C}_6\text{H}_5-\text{C}_6\text{H}_4-\text{C}_6\text{H}_4-$                                                                              | Trithiosulfo                                       | $\text{HS}-\text{S}_3-$                                                                                                                   |
| Terphenyl                              |                                                                                                                                                |                                                    |                                                                                                                                           |

TABLE 1.13 Names and Formulas of Organic Radicals (Continued)

| Name       | Formula                                                 | Name                   | Formula                                                   |
|------------|---------------------------------------------------------|------------------------|-----------------------------------------------------------|
| Trityl     | $(\text{C}_6\text{H}_5)_3\text{C}-$                     | Vanilloyl              | $3,4\text{-CH}_3\text{O}(\text{HO})\text{C}_6\text{H}_3-$ |
| Tropoyl    | $\text{C}_6\text{H}_5-\text{CH}(\text{CH}_2\text{OH})-$ |                        | $\text{CO}-$                                              |
|            | $\text{CO}-$                                            | Vanillyl               | $3,4\text{-CH}_3\text{O}(\text{HO})\text{C}_6\text{H}_3-$ |
| Tyrosyl    | $p\text{-HO}-\text{C}_6\text{H}_4-\text{CH}_2-$         |                        | $\text{CH}_2-$                                            |
|            | $\text{CH}(\text{NH}_2)-\text{CO}-$                     | Veratroyl              | $3,4\text{-(CH}_3\text{O)}_2\text{C}_6\text{H}_3-$        |
| Undecanoyl | $\text{CH}_3-[\text{CH}_2]_9-\text{CO}-$                |                        | $\text{CO}-$                                              |
| Undecyl    | $\text{CH}_3-[\text{CH}_2]_9-\text{CH}_2-$              | Veratryl               | $3,4\text{-(CH}_3\text{O)}_2\text{C}_6\text{H}_2-$        |
| Ureido     | $\text{H}_2\text{N}-\text{CO}-\text{NH}-$               |                        | $\text{CH}_2-$                                            |
| Ureylene   | $-\text{NH}-\text{CO}-\text{NH}-$                       | Vinyl                  | $\text{CH}_2=\text{CH}-$                                  |
| Valeryl    | $\text{CH}_3-[\text{CH}_2]_3-\text{CO}-$                | Vinylene               | $-\text{CH}=\text{CH}-$                                   |
| Valyl      | $(\text{CH}_3)_2\text{CH}-\text{CH}(\text{NH}_2)-$      | Xylidino (all isomers) | $(\text{CH}_3)_2\text{C}_6\text{H}_3-\text{NH}-$          |
|            | $\text{CO}-$                                            | Xylyl (all isomers)    | $(\text{CH}_3)_2\text{C}_6\text{H}_3-$                    |

1.2 PHYSICAL PROPERTIES OF PURE SUBSTANCES

TABLE 1.14 Empirical Formula Index of Organic Compounds

The alphanumeric designations are keyed to Table 1.15.

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <div>Br<sub>2</sub>OS: t149</div> <div>ClHO<sub>3</sub>S: c248</div> <div>ClH<sub>4</sub>NO: h139</div> <div>Cl<sub>2</sub>OS: t150</div> <div>Cl<sub>2</sub>H<sub>2</sub>Si: d270a</div> <div>Cl<sub>3</sub>HSi: t249</div> <div>Cl<sub>3</sub>PS: t158</div> <div>H<sub>3</sub>NO<sub>3</sub>S: s23</div> <div>H<sub>4</sub>N<sub>2</sub>: h85</div> <div>H<sub>6</sub>Si<sub>2</sub>: d791</div> <div>C<sub>1</sub></div> <div>CBr<sub>4</sub>: c13</div> <div>CBrClF<sub>2</sub>: b301</div> <div>CBrCl<sub>3</sub>: b432</div> <div>CBrF<sub>3</sub>: b434</div> <div>CBrN: c325</div> <div>CBr<sub>2</sub>F<sub>2</sub>: d93</div> <div>CBr<sub>4</sub>: c13</div> <div>CClF<sub>3</sub>: c264</div> <div>CClNO<sub>3</sub>S: c249</div> <div>CCl<sub>2</sub>F<sub>2</sub>: d218</div> <div>CCl<sub>3</sub>D: c146</div> <div>CCl<sub>3</sub>F: t237</div> <div>CCl<sub>4</sub>: c14</div> <div>CCl<sub>4</sub>S: t240</div> <div>CD<sub>2</sub>Cl<sub>2</sub>: d236</div> <div>CD<sub>4</sub>O: m36</div> <div>CD<sub>7</sub>O: m40</div> <div>CFCl<sub>3</sub>: f30</div> <div>CF<sub>4</sub>: c15</div> <div>CHBrCl<sub>2</sub>: b316</div> <div>CHBr<sub>2</sub>Cl: d88</div> | <div>CHBr<sub>2</sub>F: d104a</div> <div>CHBr<sub>3</sub>: t204</div> <div>CHClF<sub>2</sub>: c101</div> <div>CHCl<sub>2</sub>F: d233</div> <div>CHCl<sub>3</sub>: c145</div> <div>CHF<sub>3</sub>: t307</div> <div>CHF<sub>3</sub>O<sub>3</sub>S: t308</div> <div>CHI<sub>3</sub>: i33</div> <div>CH<sub>2</sub>BrCl: b305</div> <div>CH<sub>2</sub>Br<sub>2</sub>: d110</div> <div>CH<sub>2</sub>Cl<sub>2</sub>: d235</div> <div>CH<sub>2</sub>F<sub>2</sub>: d409</div> <div>CH<sub>2</sub>I<sub>2</sub>: d452</div> <div>CH<sub>3</sub>N<sub>2</sub>: c318, d63</div> <div>CH<sub>2</sub>N<sub>4</sub>: t131</div> <div>CH<sub>2</sub>O: f32</div> <div>(CH<sub>2</sub>O)<sub>x</sub>: p1</div> <div>CH<sub>2</sub>O<sub>2</sub>: f36</div> <div>CH<sub>2</sub>O<sub>3</sub>: g29</div> <div>CH<sub>2</sub>S<sub>3</sub>: t451</div> <div>CH<sub>3</sub>Br: b354</div> <div>CH<sub>3</sub>Br<sub>3</sub>Ge: m260</div> <div>CH<sub>3</sub>Cl: c157</div> <div>CH<sub>3</sub>ClO<sub>2</sub>S: m36</div> <div>CH<sub>3</sub>Cl<sub>3</sub>Si: m450, t242</div> <div>CH<sub>3</sub>DO: m39</div> <div>CH<sub>3</sub>F: f18</div> <div>CH<sub>3</sub>I: i37</div> <div>CH<sub>3</sub>NO: f33</div> <div>CH<sub>3</sub>NO<sub>2</sub>: m325, n56</div> <div>CH<sub>3</sub>NO<sub>3</sub>: m324</div> <div>CH<sub>3</sub>N<sub>5</sub>: a294</div> <div>CH<sub>4</sub>: m33</div> <div>CH<sub>4</sub>Cl<sub>2</sub>Si: d240</div> | <div>CH<sub>4</sub>N<sub>2</sub>O: f38, u16</div> <div>CH<sub>4</sub>N<sub>2</sub>S: t161</div> <div>CH<sub>4</sub>N<sub>4</sub>O<sub>2</sub>: n54</div> <div>CH<sub>4</sub>O: m38</div> <div><sup>13</sup>CH<sub>4</sub>O: m41</div> <div>CH<sub>4</sub>O<sub>2</sub>: m279</div> <div>CH<sub>4</sub>O<sub>3</sub>S: m34</div> <div>CH<sub>4</sub>S: m37</div> <div>CH<sub>3</sub>AsO<sub>3</sub>: m137</div> <div>CH<sub>3</sub>N: m127</div> <div>CH<sub>3</sub>NO<sub>3</sub>S: a201</div> <div>CH<sub>3</sub>N<sub>3</sub>: g30</div> <div>CH<sub>3</sub>N<sub>3</sub>S: t160</div> <div>CH<sub>3</sub>ClN<sub>3</sub>O: s3</div> <div>CH<sub>6</sub>N<sub>2</sub>: m274</div> <div>CH<sub>6</sub>N<sub>4</sub>: a180</div> <div>CH<sub>6</sub>N<sub>4</sub>O: c9</div> <div>Cl<sub>4</sub>: c16</div> <div>CN<sub>4</sub>O<sub>8</sub>: t123</div> <div>CS<sub>2</sub>: c10</div> <div>CO: c11</div> <div>COS: c12</div> <div>C<sub>2</sub></div> <div>C<sub>2</sub>Br<sub>2</sub>ClF<sub>3</sub>: d90</div> <div>C<sub>2</sub>Br<sub>2</sub>Cl<sub>4</sub>: d129</div> <div>C<sub>2</sub>Br<sub>2</sub>F<sub>4</sub>: d130</div> <div>C<sub>2</sub>Br<sub>2</sub>O<sub>2</sub>: o54</div> <div>C<sub>2</sub>ClF<sub>3</sub>: c263</div> <div>C<sub>2</sub>Cl<sub>2</sub>F<sub>4</sub>: d270b, d271</div> <div>C<sub>2</sub>Cl<sub>2</sub>O<sub>2</sub>: o55</div> <div>C<sub>2</sub>Cl<sub>3</sub>F<sub>3</sub>: t256, t257</div> <div>C<sub>2</sub>Cl<sub>3</sub>N: t222</div> |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|



**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                        |                                                                      |                                                                         |
|------------------------------------------------------------------------|----------------------------------------------------------------------|-------------------------------------------------------------------------|
| C <sub>2</sub> Cl <sub>4</sub> : t38                                   | C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> O: t233                | C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> : e225, g26, m187, n52    |
| C <sub>2</sub> Cl <sub>4</sub> F <sub>2</sub> : d411, d412, t36        | C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> Si: t258               | C <sub>2</sub> H <sub>5</sub> NO <sub>3</sub> : e224                    |
| C <sub>2</sub> Cl <sub>4</sub> O: t224                                 | C <sub>2</sub> H <sub>3</sub> DO <sub>2</sub> : a20                  | C <sub>2</sub> H <sub>5</sub> NS: t138                                  |
| C <sub>2</sub> Cl <sub>6</sub> : h27                                   | C <sub>2</sub> H <sub>3</sub> FO: a43                                | C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> : b238, o57 |
| C <sub>2</sub> D <sub>3</sub> N: a30                                   | C <sub>2</sub> H <sub>3</sub> FO <sub>2</sub> : f5                   | C <sub>2</sub> H <sub>6</sub> : e20                                     |
| C <sub>2</sub> D <sub>4</sub> O <sub>2</sub> : a21                     | C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O: t305                 | C <sub>2</sub> H <sub>6</sub> AlCl: d533                                |
| C <sub>2</sub> D <sub>6</sub> OS: d698                                 | C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O <sub>3</sub> S: m453  | C <sub>2</sub> H <sub>6</sub> BrN: b333                                 |
| C <sub>2</sub> F <sub>4</sub> : t65                                    | C <sub>2</sub> H <sub>3</sub> IO: a48                                | C <sub>2</sub> H <sub>6</sub> Cd: d578                                  |
| C <sub>2</sub> F <sub>6</sub> : h42                                    | C <sub>2</sub> H <sub>3</sub> IO <sub>2</sub> : i21                  | C <sub>2</sub> H <sub>6</sub> ClN: c126                                 |
| C <sub>2</sub> F <sub>6</sub> O <sub>5</sub> S <sub>2</sub> : t309     | C <sub>2</sub> H <sub>3</sub> N: a29                                 | C <sub>2</sub> H <sub>6</sub> ClNO <sub>2</sub> S: d692                 |
| C <sub>2</sub> HBrClF <sub>3</sub> : b308                              | C <sub>2</sub> H <sub>3</sub> NO: m288                               | C <sub>2</sub> H <sub>6</sub> ClO <sub>2</sub> PS: d582                 |
| C <sub>2</sub> HBr <sub>2</sub> F <sub>3</sub> : d133                  | C <sub>2</sub> H <sub>3</sub> NS: m294, m440                         | C <sub>2</sub> H <sub>6</sub> Cl <sub>3</sub> Si: d222                  |
| C <sub>2</sub> HBr <sub>2</sub> N: d77                                 | C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> : t197                  | C <sub>2</sub> H <sub>6</sub> Hg: d631                                  |
| C <sub>2</sub> HBr <sub>3</sub> : t203                                 | C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> S <sub>2</sub> : a284   | C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> : a8                       |
| C <sub>2</sub> HBr <sub>3</sub> O: t199                                | C <sub>2</sub> H <sub>4</sub> : e131                                 | C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O: m460, n78               |
| C <sub>2</sub> HBr <sub>3</sub> O <sub>2</sub> : t200                  | C <sub>2</sub> H <sub>4</sub> BrCl: b303                             | C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> : m275      |
| C <sub>2</sub> HClF <sub>2</sub> : c100a                               | C <sub>2</sub> H <sub>4</sub> BrNO: b247                             | C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> S: m444                    |
| C <sub>2</sub> HClF <sub>2</sub> O <sub>2</sub> : c98                  | C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub> : d96, d97             | C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O: o56                     |
| C <sub>2</sub> HCl <sub>3</sub> : t235                                 | C <sub>2</sub> H <sub>4</sub> ClNO: c24                              | C <sub>2</sub> H <sub>6</sub> O: d603, e27                              |
| C <sub>2</sub> HCl <sub>3</sub> O: d186, t218                          | C <sub>2</sub> H <sub>4</sub> ClO: b165a                             | C <sub>2</sub> H <sub>6</sub> OS: d697, m20                             |
| C <sub>2</sub> HCl <sub>3</sub> O <sub>2</sub> : t219                  | C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> : d225, d226           | C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> : e21a, e135               |
| C <sub>2</sub> HCl <sub>5</sub> : p7                                   | C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> O: d237                | C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> S: d696                    |
| C <sub>2</sub> HF <sub>3</sub> O <sub>2</sub> : t300                   | C <sub>2</sub> H <sub>4</sub> Cl <sub>6</sub> Si <sub>2</sub> : b227 | C <sub>2</sub> H <sub>6</sub> O <sub>3</sub> S: d695, e25, m301         |
| C <sub>2</sub> H <sub>2</sub> : a41                                    | C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> : d407                  | C <sub>2</sub> H <sub>6</sub> O <sub>4</sub> S: d693                    |
| C <sub>2</sub> H <sub>2</sub> BrClO: b255                              | C <sub>2</sub> H <sub>4</sub> INO: i20                               | C <sub>2</sub> H <sub>6</sub> O <sub>5</sub> S <sub>2</sub> : m35       |
| C <sub>2</sub> H <sub>2</sub> Br <sub>2</sub> : d99, d100              | C <sub>2</sub> H <sub>4</sub> I <sub>2</sub> : d451                  | C <sub>2</sub> H <sub>6</sub> S: d694, e26a                             |
| C <sub>2</sub> H <sub>2</sub> Br <sub>2</sub> F <sub>2</sub> : d92     | C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> : a109                  | C <sub>2</sub> H <sub>6</sub> S <sub>2</sub> : d600, e24                |
| C <sub>2</sub> H <sub>2</sub> Br <sub>2</sub> O: b254                  | C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> : o58    | C <sub>2</sub> H <sub>6</sub> Te: d700                                  |
| C <sub>2</sub> H <sub>2</sub> Br <sub>2</sub> O <sub>2</sub> : d76     | C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub> : d795   | C <sub>2</sub> H <sub>6</sub> Zn: d709                                  |
| C <sub>2</sub> H <sub>2</sub> Br <sub>4</sub> : t16                    | C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> : a289, d281            | C <sub>2</sub> H <sub>7</sub> AsO <sub>2</sub> : d560                   |
| C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub> : c262                  | C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub> : a314   | C <sub>2</sub> H <sub>7</sub> ClSi: c111                                |
| C <sub>2</sub> H <sub>2</sub> ClN: c30                                 | C <sub>2</sub> H <sub>4</sub> O: e147                                | C <sub>2</sub> H <sub>7</sub> N: d534, e63                              |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> : d227, d228, d229       | C <sub>2</sub> H <sub>4</sub> OS: t147                               | C <sub>2</sub> H <sub>7</sub> NO: a162, a163, e29                       |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O: c34                   | C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> : a19, h87, m257        | C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S: a160                   |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub> : d182    | C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> S: m16                  | C <sub>2</sub> H <sub>7</sub> NO <sub>4</sub> S: a169                   |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>3</sub> NO: t217                 | C <sub>2</sub> H <sub>4</sub> O <sub>3</sub> : h88, p60              | C <sub>2</sub> H <sub>7</sub> NS: a161                                  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub> : t36a, t37              | C <sub>2</sub> H <sub>4</sub> O <sub>5</sub> S: s26                  | C <sub>2</sub> H <sub>7</sub> N <sub>5</sub> : b137                     |
| C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> : d408                    | C <sub>2</sub> H <sub>4</sub> S: e148                                | C <sub>2</sub> H <sub>7</sub> O <sub>3</sub> P: d625                    |
| C <sub>2</sub> H <sub>2</sub> F <sub>3</sub> NO: t299                  | C <sub>2</sub> H <sub>5</sub> AlCl <sub>3</sub> : e61                | C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> : d623, d624, e21, e133    |
| C <sub>2</sub> H <sub>2</sub> F <sub>4</sub> : t64                     | C <sub>2</sub> H <sub>5</sub> Br: b329                               | C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> O: h125                    |
| C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> S <sub>2</sub> : d488     | C <sub>2</sub> H <sub>5</sub> BrNaO <sub>2</sub> S: b330             | C <sub>2</sub> H <sub>9</sub> BD: b243                                  |
| C <sub>2</sub> H <sub>2</sub> O: k1                                    | C <sub>2</sub> H <sub>5</sub> BrO: b331, b369                        | C <sub>2</sub> H <sub>10</sub> BN: b242                                 |
| C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> : g28                     | C <sub>2</sub> H <sub>5</sub> Cl: c121                               |                                                                         |
| C <sub>2</sub> H <sub>2</sub> O <sub>3</sub> : g29                     | C <sub>2</sub> H <sub>5</sub> ClHg: e198                             |                                                                         |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> : o52, o53                | C <sub>2</sub> H <sub>5</sub> ClO: c122, c156, c173                  |                                                                         |
| C <sub>2</sub> H <sub>3</sub> Br: b336                                 | C <sub>2</sub> H <sub>5</sub> ClO <sub>2</sub> : c174                |                                                                         |
| C <sub>2</sub> H <sub>3</sub> BrO: a35                                 | C <sub>2</sub> H <sub>5</sub> Cl <sub>2</sub> OPS: e124              |                                                                         |
| C <sub>2</sub> H <sub>3</sub> BrO <sub>2</sub> : b249                  | C <sub>2</sub> H <sub>5</sub> Cl <sub>2</sub> O <sub>2</sub> P: e123 |                                                                         |
| C <sub>2</sub> H <sub>3</sub> Br <sub>2</sub> Cl <sub>3</sub> Si: d101 | C <sub>2</sub> H <sub>5</sub> Cl <sub>3</sub> Si: c171, e269, t236   |                                                                         |
| C <sub>2</sub> H <sub>3</sub> Br <sub>3</sub> O: t202                  | C <sub>2</sub> H <sub>5</sub> DO: e28                                |                                                                         |
| C <sub>2</sub> H <sub>3</sub> Cl: c129                                 | C <sub>2</sub> H <sub>5</sub> F: f17                                 |                                                                         |
| C <sub>2</sub> H <sub>3</sub> ClF <sub>2</sub> : c100                  | C <sub>2</sub> H <sub>5</sub> I: i31                                 |                                                                         |
| C <sub>2</sub> H <sub>3</sub> ClO: a37, c23a                           | C <sub>2</sub> H <sub>5</sub> IO: i32                                |                                                                         |
| C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub> : c27, m194             | C <sub>2</sub> H <sub>5</sub> N: e146                                |                                                                         |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> : t231, t232             | C <sub>2</sub> H <sub>5</sub> NO: a5, a6, m255, m291                 |                                                                         |
|                                                                        |                                                                      | C <sub>3</sub>                                                          |
|                                                                        |                                                                      | C <sub>3</sub> Br <sub>2</sub> F <sub>5</sub> : d105                    |
|                                                                        |                                                                      | C <sub>3</sub> Cl <sub>3</sub> N <sub>3</sub> : t255                    |
|                                                                        |                                                                      | C <sub>3</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>3</sub> : t239     |
|                                                                        |                                                                      | C <sub>3</sub> Cl <sub>6</sub> : h30                                    |
|                                                                        |                                                                      | C <sub>3</sub> Cl <sub>6</sub> O: a27, h2                               |
|                                                                        |                                                                      | C <sub>3</sub> F <sub>6</sub> : h44                                     |
|                                                                        |                                                                      | C <sub>3</sub> HCl <sub>5</sub> O: p5                                   |
|                                                                        |                                                                      | C <sub>3</sub> H <sub>2</sub> ClN: c35                                  |
|                                                                        |                                                                      | C <sub>3</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub> : m6       |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| C <sub>3</sub> H <sub>2</sub> Cl <sub>4</sub> O: t31<br>C <sub>3</sub> H <sub>2</sub> Cl <sub>4</sub> O <sub>2</sub> : t234<br>C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O: h43<br>C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> : m5<br>C <sub>3</sub> H <sub>2</sub> O <sub>2</sub> : p248<br>C <sub>3</sub> H <sub>3</sub> Br: b415<br>C <sub>3</sub> H <sub>3</sub> Br <sub>2</sub> N: d126<br>C <sub>3</sub> H <sub>3</sub> Cl: c241<br>C <sub>3</sub> H <sub>3</sub> ClO: a63a<br>C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub> O: e18, t221<br>C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub> O <sub>2</sub> : m449<br>C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O: t302<br>C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O <sub>2</sub> : m452<br>C <sub>3</sub> H <sub>3</sub> N: a63<br>C <sub>3</sub> H <sub>3</sub> NOS <sub>2</sub> : r7<br>C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> : c320<br>C <sub>3</sub> H <sub>3</sub> NS: t136<br>C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S: a244<br>C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>3</sub> : a289, c332<br>C <sub>3</sub> H <sub>4</sub> : a72, p246<br>C <sub>3</sub> H <sub>4</sub> BrClO: b410, b411<br>C <sub>3</sub> H <sub>4</sub> BrN: b408<br>C <sub>3</sub> H <sub>4</sub> Br <sub>2</sub> : d124<br>C <sub>3</sub> H <sub>4</sub> Br <sub>2</sub> O: b409<br>C <sub>3</sub> H <sub>4</sub> Br <sub>2</sub> O <sub>2</sub> : d125<br>C <sub>3</sub> H <sub>4</sub> ClN: c233<br>C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> : d265, d266<br>C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O: c235, c236, d183, d184<br>C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub> : m227<br>C <sub>3</sub> H <sub>4</sub> F <sub>4</sub> O: t66<br>C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> : i3, m241, p254<br>C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O: c287<br>C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> : h84<br>C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S: a285<br>C <sub>3</sub> H <sub>4</sub> N <sub>3</sub> NaS: c326<br>C <sub>3</sub> H <sub>4</sub> O: p203, p249<br>C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> : a62, o64<br>C <sub>3</sub> H <sub>4</sub> O <sub>3</sub> : e132, o65, p210<br>C <sub>3</sub> H <sub>4</sub> O <sub>4</sub> : m3<br>C <sub>3</sub> H <sub>4</sub> Br: b314, b404, b405<br>C <sub>3</sub> H <sub>3</sub> BrO: b328, b403<br>C <sub>3</sub> H <sub>3</sub> BrO <sub>2</sub> : b406, b407, m143<br>C <sub>3</sub> H <sub>3</sub> Br <sub>3</sub> : t206<br>C <sub>3</sub> H <sub>5</sub> Cl: c236a<br>C <sub>3</sub> H <sub>5</sub> ClO: c120, c232, p216<br>C <sub>3</sub> H <sub>5</sub> ClO <sub>2</sub> : c228, c229, e109, m188<br>C <sub>3</sub> H <sub>5</sub> Cl <sub>3</sub> : t247<br>C <sub>3</sub> H <sub>5</sub> Cl <sub>3</sub> Si: a98<br>C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> O <sub>3</sub> S: m453<br>C <sub>3</sub> H <sub>5</sub> I: a87, i50<br>C <sub>3</sub> H <sub>5</sub> N: p215<br>C <sub>3</sub> H <sub>5</sub> NO: c323, h172, h173, v11 | C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub> : o59<br>C <sub>3</sub> H <sub>5</sub> NS: e193, m435<br>C <sub>3</sub> H <sub>5</sub> NS <sub>2</sub> : m26<br>C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O: c321<br>C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>3</sub> : g22<br>C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> S: c293<br>C <sub>3</sub> H <sub>6</sub> : c406, p204<br>C <sub>3</sub> H <sub>6</sub> BrCl: b307<br>C <sub>3</sub> H <sub>6</sub> BrNO <sub>3</sub> : b381<br>C <sub>3</sub> H <sub>6</sub> Br <sub>2</sub> : d120, d121<br>C <sub>3</sub> H <sub>6</sub> Br <sub>2</sub> O: d122, d123<br>C <sub>3</sub> H <sub>6</sub> ClI: c155<br>C <sub>3</sub> H <sub>6</sub> ClNO: d578<br>C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> : d262, d263<br>C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> : d173<br>C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> O: d231, d264<br>C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> Si: d241<br>C <sub>3</sub> H <sub>6</sub> Cl <sub>4</sub> Si: t230<br>C <sub>3</sub> H <sub>6</sub> I <sub>2</sub> : d454<br>C <sub>3</sub> H <sub>6</sub> NO: a61<br>C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> : d583<br>C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O: i5<br>C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> : m4<br>C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> OS: a58<br>C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> : m4, m270<br>C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S: a286, i4<br>C <sub>3</sub> H <sub>6</sub> O: a26, a78, e15, m462, p211, p232<br>C <sub>3</sub> H <sub>6</sub> OS: t159<br>C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> : d734, e16, e154, h90, m122, p213<br>C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S: m22, m23, m298<br>C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> : d445, d580, L1, L2, m43, m265, t407<br>C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> S: p197<br>C <sub>3</sub> H <sub>6</sub> S: p205, p233<br>C <sub>3</sub> H <sub>6</sub> S <sub>3</sub> : t450<br>C <sub>3</sub> H <sub>7</sub> Br: b400, b401<br>C <sub>3</sub> H <sub>7</sub> BrO: b402<br>C <sub>3</sub> H <sub>7</sub> Cl: c172, c225, c226<br>C <sub>3</sub> H <sub>7</sub> ClO: c132, c153, c230, c231<br>C <sub>3</sub> H <sub>7</sub> CLOS: c156<br>C <sub>3</sub> H <sub>7</sub> ClO <sub>2</sub> : c227<br>C <sub>3</sub> H <sub>7</sub> ClO <sub>2</sub> S: p196<br>C <sub>3</sub> H <sub>7</sub> Cl <sub>2</sub> OP: p241<br>C <sub>3</sub> H <sub>7</sub> Cl <sub>3</sub> Si: d214, p242<br>C <sub>3</sub> H <sub>7</sub> I: i48, i49<br>C <sub>3</sub> H <sub>7</sub> N: a76, p231<br>C <sub>3</sub> H <sub>7</sub> NO: a28, d606, m120, p212<br>C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> : a68, a69, a70, e102, i125, m264, n73, n74<br>C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S: c411<br>C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> : i124, n75, p238, s4 | C <sub>3</sub> H <sub>7</sub> NS: d704<br>C <sub>3</sub> H <sub>8</sub> : p188<br>C <sub>3</sub> H <sub>8</sub> BrClSi: b366<br>C <sub>3</sub> H <sub>8</sub> ClN: c225<br>C <sub>3</sub> H <sub>8</sub> Cl <sub>2</sub> Si: c88, d232<br>C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O: d708, e274<br>C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> : e103<br>C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> S: d705<br>C <sub>3</sub> H <sub>8</sub> O: e10, e210, p201, p202<br>C <sub>3</sub> H <sub>8</sub> OS <sub>2</sub> : d485, m315<br>C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> : d507, m71, p191, p192<br>C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> S: m21<br>C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> : g19<br>C <sub>3</sub> H <sub>8</sub> S: e221, p198, p199<br>C <sub>3</sub> H <sub>8</sub> S <sub>2</sub> : p195<br>C <sub>3</sub> H <sub>9</sub> Al: t352<br>C <sub>3</sub> H <sub>9</sub> BO <sub>3</sub> : t338<br>C <sub>3</sub> H <sub>9</sub> B <sub>3</sub> O <sub>6</sub> : t339<br>C <sub>3</sub> H <sub>9</sub> BrGe: b437<br>C <sub>3</sub> H <sub>9</sub> BrSi: b438<br>C <sub>3</sub> H <sub>9</sub> ClGe: c265<br>C <sub>3</sub> H <sub>9</sub> ClSi: c266<br>C <sub>3</sub> H <sub>9</sub> IOS: t400<br>C <sub>3</sub> H <sub>9</sub> IS: t399<br>C <sub>3</sub> H <sub>9</sub> ISi: i56<br>C <sub>3</sub> H <sub>9</sub> N: i100, p223, t354<br>C <sub>3</sub> H <sub>9</sub> NO: a263, a264, a265, a266, m77, m131<br>C <sub>3</sub> H <sub>9</sub> NO <sub>2</sub> : a262<br>C <sub>3</sub> H <sub>9</sub> N <sub>3</sub> Si: a309<br>C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> P: d635, t390<br>C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P: t389<br>C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> : d54, d55, m254, p189, p190<br>C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O: d56<br>C <sub>3</sub> H <sub>10</sub> O <sub>3</sub> Si: t343<br>C <sub>3</sub> H <sub>11</sub> Br <sub>2</sub> N <sub>3</sub> S: a171 |
| C <sub>4</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| C <sub>4</sub> Cl <sub>6</sub> : h23<br>C <sub>4</sub> Cl <sub>6</sub> O <sub>3</sub> : t220<br>C <sub>4</sub> D <sub>6</sub> O <sub>3</sub> : a23<br>C <sub>4</sub> F <sub>6</sub> O <sub>3</sub> : t301<br>C <sub>4</sub> HBrO <sub>3</sub> : b352<br>C <sub>4</sub> HCl <sub>3</sub> N <sub>2</sub> : t248<br>C <sub>4</sub> HF <sub>7</sub> O <sub>2</sub> : h2<br>C <sub>4</sub> H <sub>2</sub> : b452<br>C <sub>4</sub> H <sub>2</sub> Br <sub>2</sub> S: d131<br>C <sub>4</sub> H <sub>2</sub> Cl <sub>3</sub> N <sub>2</sub> : d267<br>C <sub>4</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub> : f43<br>C <sub>4</sub> H <sub>2</sub> Cl <sub>2</sub> S: d272<br>C <sub>4</sub> H <sub>2</sub> F <sub>6</sub> O <sub>2</sub> : t306<br>C <sub>4</sub> H <sub>2</sub> O <sub>3</sub> : m2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                      |                                                                                                                    |                                                                                                                    |
|--------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|
| C <sub>4</sub> H <sub>2</sub> O <sub>4</sub> : q42                                   | C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> : a149, m284, m285, m286                                              | C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> : b480, b481, b614, d732, d733, e57, h107, h108, i81. m64, m401, p234 |
| C <sub>4</sub> H <sub>3</sub> IS: i52                                                | C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> : e121, m273                                           | C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S: e196, m299, t107                                                   |
| C <sub>4</sub> H <sub>3</sub> N <sub>3</sub> O <sub>4</sub> : n88                    | C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S: a225                                                               | C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> : e24, e153, h120, h138, m70, m296, m302                              |
| C <sub>4</sub> H <sub>4</sub> : b489                                                 | C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub> : d584                                                 | C <sub>4</sub> H <sub>8</sub> S: a90, t87                                                                          |
| C <sub>4</sub> H <sub>4</sub> BrNO <sub>2</sub> : b422                               | C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O: d39                                                                | C <sub>4</sub> H <sub>8</sub> S <sub>2</sub> : d792                                                                |
| C <sub>4</sub> H <sub>4</sub> Br <sub>2</sub> O <sub>2</sub> : d86                   | C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub> : a71                                                  | C <sub>4</sub> H <sub>9</sub> Br: b274, b275, b371, b372                                                           |
| C <sub>4</sub> H <sub>4</sub> Br <sub>2</sub> O <sub>4</sub> : d128                  | C <sub>4</sub> H <sub>6</sub> O: b488, c306, d421, m27, m407                                                       | C <sub>4</sub> H <sub>9</sub> BrO: b337                                                                            |
| C <sub>4</sub> H <sub>4</sub> ClNO <sub>2</sub> : c247                               | C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> : b466, b483, b484, b485, b611, b616, b617, c307, c409, m29, m126, v5 | C <sub>4</sub> H <sub>9</sub> BrO <sub>2</sub> : b319                                                              |
| C <sub>4</sub> H <sub>4</sub> ClO <sub>3</sub> : c28                                 | C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> S: b450                                                               | C <sub>4</sub> H <sub>9</sub> Cl: c75, c76, c179, c180                                                             |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> : d213                                 | C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> : a22, a24, m355, o60, p230                                           | C <sub>4</sub> H <sub>9</sub> ClO: a64, c77, c131, m74                                                             |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub> : s19                   | C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> : d652, s15                                                           | C <sub>4</sub> H <sub>9</sub> ClO <sub>2</sub> : c105, c123, m67                                                   |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>3</sub> : c25                   | C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> S: m25, t143                                                          | C <sub>4</sub> H <sub>9</sub> ClSi: c112                                                                           |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> : b456, p251, p256, p277, s18           | C <sub>4</sub> H <sub>6</sub> O <sub>5</sub> : d690, h186, h187, o67                                               | C <sub>4</sub> H <sub>9</sub> Cl <sub>3</sub> Si: b604, b603, d215                                                 |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> : d448, p278             | C <sub>4</sub> H <sub>6</sub> O <sub>6</sub> : t1, t2, t3, t4                                                      | C <sub>4</sub> H <sub>9</sub> Cl <sub>3</sub> Sn: b600                                                             |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S: d437                  | C <sub>4</sub> H <sub>7</sub> Br: b276, b277, b278                                                                 | C <sub>4</sub> H <sub>9</sub> F: f21                                                                               |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> : b1                     | C <sub>4</sub> H <sub>7</sub> BrO <sub>2</sub> : b282, b332, b368, b373, e83, m156                                 | C <sub>4</sub> H <sub>9</sub> I: i26, i27, i38, i39                                                                |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>5</sub> : a73                    | C <sub>4</sub> H <sub>7</sub> Cl: c79, c80, c81, c181, c182, c312                                                  | C <sub>4</sub> H <sub>9</sub> N: e53, p280                                                                         |
| C <sub>4</sub> H <sub>4</sub> N <sub>4</sub> : d50                                   | C <sub>4</sub> H <sub>7</sub> ClO: b620, c78, c136, i85                                                            | C <sub>4</sub> H <sub>9</sub> NO: a311, b476, b613, d526, i80, m110, m463                                          |
| C <sub>4</sub> H <sub>4</sub> O: f45                                                 | C <sub>4</sub> H <sub>7</sub> ClO <sub>2</sub> : c84, c85, e105, m196, p228                                        | C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> : a133, a133a, a134, b578, b579, h119, i73, n48                      |
| C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> : d483                                  | C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> O: t241                                                              | C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S: a200                                                              |
| C <sub>4</sub> H <sub>4</sub> O <sub>3</sub> : s16                                   | C <sub>4</sub> H <sub>7</sub> FO <sub>2</sub> : e153                                                               | C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub> : a185, a186, i72, m341, n49                                         |
| C <sub>4</sub> H <sub>4</sub> O <sub>4</sub> : f42, m1                               | C <sub>4</sub> H <sub>7</sub> N: b618, i83                                                                         | C <sub>4</sub> H <sub>9</sub> NO <sub>5</sub> : t442                                                               |
| C <sub>4</sub> H <sub>4</sub> S: t151                                                | C <sub>4</sub> H <sub>7</sub> NO: h153, i115, m28, m99a, m352, p236, p285                                          | C <sub>4</sub> H <sub>9</sub> NSi: c331                                                                            |
| C <sub>4</sub> H <sub>4</sub> BrO <sub>2</sub> : b283                                | C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> : b467, h146, m351                                                   | C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> : c301                                                 |
| C <sub>4</sub> H <sub>4</sub> BrO <sub>4</sub> : b421                                | C <sub>4</sub> H <sub>7</sub> NO <sub>3</sub> : a46, e233, s13                                                     | C <sub>4</sub> H <sub>10</sub> : b454, m390                                                                        |
| C <sub>4</sub> H <sub>4</sub> Cl: c74, c74a, c83                                     | C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub> : a304, i7                                                           | C <sub>4</sub> H <sub>10</sub> AlCl: d320, e62                                                                     |
| C <sub>4</sub> H <sub>4</sub> ClN <sub>2</sub> O <sub>2</sub> : c184                 | C <sub>4</sub> H <sub>7</sub> NS: m434                                                                             | C <sub>4</sub> H <sub>10</sub> ClO <sub>2</sub> PS: d351                                                           |
| C <sub>4</sub> H <sub>4</sub> ClO: c310, c408, m31                                   | C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O: c302                                                               | C <sub>4</sub> H <sub>10</sub> ClO <sub>3</sub> P: d350                                                            |
| C <sub>4</sub> H <sub>4</sub> ClO <sub>2</sub> : a82                                 | C <sub>4</sub> H <sub>8</sub> : b477, b478, b479, c333, m399                                                       | C <sub>4</sub> H <sub>10</sub> Cl <sub>2</sub> Si: b165                                                            |
| C <sub>4</sub> H <sub>4</sub> ClO <sub>3</sub> : c194, e232                          | C <sub>4</sub> H <sub>8</sub> BrCl: b298, b306                                                                     | C <sub>4</sub> H <sub>10</sub> Cl <sub>4</sub> Si <sub>2</sub> : b174                                              |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>3</sub> O <sub>2</sub> : e268                  | C <sub>4</sub> H <sub>8</sub> Br <sub>2</sub> : d81, d82, d83, d84                                                 | C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> : p178                                                               |
| C <sub>4</sub> H <sub>4</sub> N: b482, c309, c407, m30a, p279                        | C <sub>4</sub> H <sub>8</sub> Br <sub>2</sub> O: b148                                                              | C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O: a227                                                              |
| C <sub>4</sub> H <sub>4</sub> NO: m47, m295                                          | C <sub>4</sub> H <sub>8</sub> Br <sub>2</sub> O <sub>2</sub> : d85                                                 | C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> S: a8                                                 |
| C <sub>4</sub> H <sub>4</sub> NO <sub>2</sub> : m201, s17                            | C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> : d210                                                               | C <sub>4</sub> H <sub>10</sub> O: b473, b474, d365, m397, m398, m404                                               |
| C <sub>4</sub> H <sub>4</sub> NO <sub>2</sub> S: e39                                 | C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O: b163, d230                                                        | C <sub>4</sub> H <sub>10</sub> OS: e180                                                                            |
| C <sub>4</sub> H <sub>4</sub> NO <sub>3</sub> : h183                                 | C <sub>4</sub> H <sub>8</sub> I <sub>2</sub> : d450                                                                | C <sub>4</sub> H <sub>10</sub> OS <sub>2</sub> : b208                                                              |
| C <sub>4</sub> H <sub>4</sub> NS: a88, m432                                          | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> : d535                                                                | C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> : b457, b457a, b457b, b458, b563, d504, d505, e40, e141, m105, m393  |
| C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> : a278, i8                              | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O: a102                                                               | C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> S: t144                                                              |
| C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> O: a194                                 | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> : d610, s14                                            | C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> S <sub>2</sub> : d484, h123                                          |
| C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> OS: a187                                | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> : a313, g27                                            | C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> : b198, b472, d361, o62, t378                                        |
| C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> O <sub>2</sub> : a152, a153, c322, m338 | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S: a97, t85                                                           | C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> S: d399                                                              |
| C <sub>4</sub> H <sub>4</sub> N <sub>4</sub> O: d49                                  | C <sub>4</sub> H <sub>8</sub> O: b475, b486, b487, b612, c311, e3, e276, i79, m106, m389, m400, t69                | C <sub>4</sub> H <sub>10</sub> O <sub>4</sub> : e19                                                                |
| C <sub>4</sub> H <sub>4</sub> : b448, b449, b610a, b610b                             |                                                                                                                    | C <sub>4</sub> H <sub>10</sub> O <sub>4</sub> S: d397                                                              |
| C <sub>4</sub> H <sub>4</sub> Br <sub>2</sub> O: b374                                |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub> : d95    |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> Br <sub>2</sub> O <sub>2</sub> : d87                   |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> ClN: c86                                               |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> : c89, d211, d212                      |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O: c87                                 |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub> : m229                  |                                                                                                                    |                                                                                                                    |
| C <sub>4</sub> H <sub>4</sub> Cl <sub>3</sub> NSi: t250                              |                                                                                                                    |                                                                                                                    |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p> <math>C_4H_{10}S</math>: b470, b471, d398, i104, m394, m395, m396, m406<br/> <math>C_4H_{10}S_2</math>: b468, d356<br/> <math>C_4H_{10}S_3</math>: b209<br/> <math>C_4H_{10}Zn</math>: d405<br/> <math>C_4H_{11}ClSi</math>: c183<br/> <math>C_4H_{11}N</math>: b453, b509, b510, b511, d323, d604, i66, m293<br/> <math>C_4H_{11}NO</math>: a135, a164, a203, a216, d376, d539, e44, e67, m112<br/> <math>C_4H_{11}NO_2</math>: a215, d297, d506<br/> <math>C_4H_{11}NO_3</math>: t439<br/> <math>C_4H_{11}OP</math>: d390<br/> <math>C_4H_{11}O_2PS_2</math>: d358<br/> <math>C_4H_{11}O_3P</math>: d375<br/> <math>C_4H_{12}BrN</math>: t93<br/> <math>C_4H_{12}ClN</math>: d324, t94<br/> <math>C_4H_{12}Ge</math>: t109<br/> <math>C_4H_{12}IN</math>: t95<br/> <math>C_4H_{12}N_2</math>: b455, b560, b562, d41, d605, m391, m392<br/> <math>C_4H_{12}N_2O</math>: a165<br/> <math>C_4H_{12}N_2S_4</math>: b183<br/> <math>C_4H_{12}OSi</math>: m119<br/> <math>C_4H_{12}O_2Si</math>: d502<br/> <math>C_4H_{12}O_3Si</math>: m455<br/> <math>C_4H_{12}Pb</math>: t112<br/> <math>C_4H_{12}Si</math>: t118<br/> <math>C_4H_{12}Sn</math>: t121<br/> <math>C_4H_{13}N_3</math>: d362<br/> <math>C_4H_{14}BN</math>: b239<br/> <math>C_4H_{14}OSi_2</math>: t106<br/> <math>C_4H_{16}O_4Si_4</math>: t104 </p> | <p> <math>C_5H_4O_2</math>: f44<br/> <math>C_5H_4O_2S</math>: t155<br/> <math>C_5H_4O_3</math>: c285, f54<br/> <math>C_5H_5ClN_2</math>: a148<br/> <math>C_5H_5ClN_2O_2</math>: c168<br/> <math>C_5H_5N</math>: p257<br/> <math>C_5H_5NO</math>: h179, h180, h181, p271<br/> <math>C_5H_5NO_2</math>: d448, h183<br/> <math>C_5H_5N_3O_2</math>: a243<br/> <math>C_5H_5N_3O_4</math>: a158<br/> <math>C_5H_5N_5</math>: a61<br/> <math>C_5H_6</math>: c395, m174<br/> <math>C_5H_6BrClN_2O_2</math>: b302<br/> <math>C_5H_6Br_2N_2O_2</math>: d76<br/> <math>C_5H_6Cl_2NO_2</math>: d220<br/> <math>C_5H_6Cl_2O_2</math>: g18<br/> <math>C_5H_6N_2</math>: a275, a276, a277, g17, m408, v12<br/> <math>C_5H_6N_2O</math>: a47, a193<br/> <math>C_5H_6N_2OS</math>: h140, h141<br/> <math>C_5H_6O</math>: m259<br/> <math>C_5H_6OS</math>: f48, m443<br/> <math>C_5H_6O_2</math>: f50<br/> <math>C_5H_6O_3</math>: g15, h156<br/> <math>C_5H_6O_4</math>: c284, m253<br/> <math>C_5H_6O_4S_3</math>: b156<br/> <math>C_5H_6S</math>: m441, m442<br/> <math>C_5H_7BN</math>: b244<br/> <math>C_5H_7BrO_3</math>: e91<br/> <math>C_5H_7ClO_2</math>: c205, d581<br/> <math>C_5H_7ClO_3</math>: m189, m190, m195<br/> <math>C_5H_7N</math>: m417, p51, p52<br/> <math>C_5H_7NO</math>: e31, f51<br/> <math>C_5H_7NO_2</math>: c324, e115<br/> <math>C_5H_7N_3</math>: a224, d58<br/> <math>C_5H_7N_3O</math>: a188<br/> <math>C_5H_8</math>: c401, d424, m157, m178, p15, p16, p17, p18, p58<br/> <math>C_5H_8Br_2O_2</math>: e122<br/> <math>C_5H_8N_2</math>: d626, d684, e191, p283<br/> <math>C_5H_8N_2O_2</math>: d622<br/> <math>C_5H_8N_4O_{12}</math>: p22<br/> <math>C_5H_8O</math>: c399, c410, d364, e6, m179<br/> <math>C_5H_8O_2</math>: a74, c334, d532, e60, g16, i95, m65, m168, m169, m170, m200, m225, m300, p33, p34, p207, v2, v3, v10, v14<br/> <math>C_5H_8O_3</math>: e237, h121, m123, o63<br/> <math>C_5H_8O_4</math>: d547, g14, m278 </p> | <p> <math>C_5H_9Br</math>: b313, b365<br/> <math>C_5H_9BrO_2</math>: b364, e93, e94, m155<br/> <math>C_5H_9Cl</math>: c93<br/> <math>C_5H_9ClO</math>: c206, d681, m186, p45, t75, t351<br/> <math>C_5H_9ClOS</math>: c238<br/> <math>C_5H_9ClO_2</math>: b538, c237, e110, e111, i68, i107, m193<br/> <math>C_5H_9N</math>: d683, m185, p35<br/> <math>C_5H_9NO</math>: b565, b566, c400, d531, e53, e234, m419, m461<br/> <math>C_5H_9NO_2</math>: d523, f39, m130, p187<br/> <math>C_5H_9NO_4</math>: g12<br/> <math>C_5H_{10}</math>: c396, m165a, m166, m167, p48, p49, p50<br/> <math>C_5H_{10}Br_2</math>: d117, d118<br/> <math>C_5H_{10}ClNO</math>: d348<br/> <math>C_5H_{10}Cl_2</math>: d209<br/> <math>C_5H_{10}Cl_2</math>: d251<br/> <math>C_5H_{10}I_2</math>: d453<br/> <math>C_5H_{10}NO_3P</math>: d293a<br/> <math>C_5H_{10}N_2</math>: d548<br/> <math>C_5H_{10}N_2O</math>: d627<br/> <math>C_5H_{10}N_2O_3</math>: g13<br/> <math>C_5H_{10}N_2O_4S_2</math>: c412<br/> <math>C_5H_{10}O</math>: a85, c398, d653, d677, e252, m165, m171, m172, m173, m180, m181, m429, p28, p42, p43, t83<br/> <math>C_5H_{10}OS</math>: m439<br/> <math>C_5H_{10}O_2</math>: b557, c398, d521, d679, e252, h147, h164, i69, i99, m86, m182, m183, m184, m237, m290, m353, p38, p222, t71, t349<br/> <math>C_5H_{10}O_2S</math>: e197, e222, m316, m431<br/> <math>C_5H_{10}O_3</math>: d349, d520, e194, m75, m282, m307<br/> <math>C_5H_{10}O_4</math>: b201, m72<br/> <math>C_5H_{10}O_5</math>: a300, r9, x8<br/> <math>C_5H_{11}Br</math>: b362, b363, b387, b388<br/> <math>C_5H_{11}BrO</math>: b322<br/> <math>C_5H_{11}BrO_2</math>: b320<br/> <math>C_5H_{11}Br_2O</math>: b148<br/> <math>C_5H_{11}Br_2O_2</math>: b150<br/> <math>C_5H_{11}Cl</math>: c109, c150, c169a, c170, c204a<br/> <math>C_5H_{11}ClO</math>: c110<br/> <math>C_5H_{11}Cl_2N</math>: b164<br/> <math>C_5H_{11}I</math>: i47 </p> |
| <p> <math>C_5</math> </p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| <p> <math>C_5Cl_5N</math>: p10<br/> <math>C_5Cl_6</math>: h25<br/> <math>C_5D_5N</math>: p258<br/> <math>C_5H_3BrS</math>: b426, b427<br/> <math>C_5H_3Br_2N</math>: d127<br/> <math>C_5H_3ClOS</math>: t153<br/> <math>C_5H_3ClO_2</math>: f55<br/> <math>C_5H_3ClS</math>: c251<br/> <math>C_5H_3Cl_2N</math>: d268, d269<br/> <math>C_5H_3N_3</math>: p252<br/> <math>C_5H_4BrN</math>: b416, b417<br/> <math>C_5H_4ClN</math>: c242<br/> <math>C_5H_4FN</math>: f26<br/> <math>C_5H_4F_8O</math>: o20<br/> <math>C_5H_4N_2O_2</math>: p253<br/> <math>C_5H_4N_2O_3</math>: n76<br/> <math>C_5H_4N_4O_3</math>: u17<br/> <math>C_5H_4OS</math>: t154 </p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p> <math>C_5H_{11}N</math>: a85, c404, m418, p180<br/> <math>C_5H_{11}NO</math>: b558, d369, d678, m317, t72<br/> <math>C_5H_{11}NO_2</math>: a248, a249, b133, b532, e275, i92, m310a, v4<br/> <math>C_5H_{11}NO_2S</math>: m42<br/> <math>C_5H_{11}NO_3</math>: n58<br/> <math>C_5H_{11}NS_2</math>: d357<br/> <math>C_5H_{11}O_3P</math>: t391<br/> <math>C_5H_{12}</math>: d673, m155, p29<br/> <math>C_5H_{12}Cl_2O_2Si</math>: b162<br/> <math>C_5H_{12}N_2</math>: a261, m381, m382<br/> <math>C_5H_{12}N_2O</math>: b608, d702, t122<br/> <math>C_5H_{12}N_2O_2</math>: b533, o46<br/> <math>C_5H_{12}N_2S</math>: t119<br/> <math>C_5H_{12}N_2S_2</math>: p282<br/> <math>C_5H_{12}O</math>: b572, d676, e254, m161, m162, m163, m164, p31, p32, p39, p40, p41<br/> <math>C_5H_{12}O_2</math>: b504, d307, d518, d519, d675, i97, m64, p218<br/> <math>C_5H_{12}O_2Si</math>: d509, t395, v18<br/> <math>C_5H_{12}O_3</math>: m73, t340, t377, t440<br/> <math>C_5H_{12}O_3S</math>: p36<br/> <math>C_5H_{12}O_4</math>: p19<br/> <math>C_5H_{12}O_5</math>: x7<br/> <math>C_5H_{12}S</math>: b577, e255, m159, m160, p37<br/> <math>C_5H_{12}Si</math>: t401<br/> <math>C_5H_{13}ClOSi</math>: c125<br/> <math>C_5H_{13}N</math>: a246, a247, d380, d628, d682, m175, m176, p54<br/> <math>C_5H_{13}NO</math>: a209, a250, d546, d547, e54, p224<br/> <math>C_5H_{13}NOSi</math>: t394<br/> <math>C_5H_{13}NO_2</math>: a176, d508, d545, d607, m230<br/> <math>C_5H_{13}N_3</math>: t110<br/> <math>C_5H_{14}ClN_3O</math>: g5<br/> <math>C_5H_{14}N_2</math>: d549, d674, p30, t105, t113<br/> <math>C_5H_{14}N_2O</math>: a150, a166<br/> <math>C_5H_{14}O</math>: b560, b561<br/> <math>C_5H_{14}OSi</math>: e56<br/> <math>C_5H_{15}NSi</math>: d707<br/> <math>C_5H_{15}N_3</math>: a175 </p> | <p> <math>C_6Cl_6</math>: h22<br/> <math>C_6D_6</math>: b11<br/> <math>C_6D_{12}</math>: c348<br/> <math>C_6F_6</math>: h41<br/> <math>C_6F_{14}</math>: t42<br/> <math>C_6HBr_5O</math>: p4<br/> <math>C_6HCl_4NO_2</math>: t39<br/> <math>C_6HCl_5</math>: p6<br/> <math>C_6HCl_5O</math>: p9<br/> <math>C_6H_2BrFN_2O_4</math>: b324<br/> <math>C_6H_2Br_4</math>: t14<br/> <math>C_6H_2Cl_3NO_2</math>: t243<br/> <math>C_6H_2Cl_4</math>: t32, t33<br/> <math>C_6H_3Br_2F</math>: d103, d104<br/> <math>C_6H_3Br_2NO_2</math>: d115<br/> <math>C_6H_3Br_3O</math>: t211<br/> <math>C_6H_3ClFNO_2</math>: c141<br/> <math>C_6H_3ClF_2</math>: c99<br/> <math>C_6H_3ClN_2O_4</math>: c114, c115<br/> <math>C_6H_3ClN_2O_5S</math>: d712<br/> <math>C_6H_3Cl_2NO_2</math>: d245, d246, d247, d248<br/> <math>C_6H_3Cl_2NO_3</math>: d249<br/> <math>C_6H_3Cl_3</math>: t227, t228, t229<br/> <math>C_6H_3Cl_3O</math>: t244, t245<br/> <math>C_6H_3Cl_3O_2S</math>: d201<br/> <math>C_6H_3D_3</math>: b9<br/> <math>C_6H_3FN_2O_4</math>: d718<br/> <math>C_6H_3F_2NO_2</math>: d410<br/> <math>C_6H_3F_3</math>: t303<br/> <math>C_6H_3N_3O_6</math>: t403, t404<br/> <math>C_6H_3N_3O_7</math>: p174<br/> <math>C_6H_4BrCl</math>: b287, b288, b296<br/> <math>C_6H_4BrClO_2S</math>: b264<br/> <math>C_6H_4BrF</math>: b340, b341, b342<br/> <math>C_6H_4BrNO_2</math>: b378<br/> <math>C_6H_4BrN_3O_4</math>: b323<br/> <math>C_6H_4Br_2</math>: d79, d112<br/> <math>C_6H_4Br_2N_2O_2</math>: d114<br/> <math>C_6H_4Br_2O</math>: d119<br/> <math>C_6H_4Br_3N</math>: t201<br/> <math>C_6H_4ClF</math>: c137, c138<br/> <math>C_6H_4ClFO</math>: c142<br/> <math>C_6H_4ClI</math>: c154<br/> <math>C_6H_4ClNO_2</math>: c192, c193, c194<br/> <math>C_6H_4ClNO_3</math>: c201<br/> <math>C_6H_4ClNO_4S</math>: n33<br/> <math>C_6H_4Cl_2</math>: d198, d199, d200<br/> <math>C_6H_4Cl_2N_2O_2</math>: d244<br/> <math>C_6H_4Cl_2O</math>: d252, d253, d254, d255<br/> <math>C_6H_4Cl_2O_2S</math>: c50<br/> <math>C_6H_4Cl_3N</math>: t225, t226<br/> <math>C_6H_4FNO_2</math>: f23<br/> <math>C_6H_4F_2</math>: d406 </p> | <p> <math>C_6H_4INO_2</math>: i40, i41<br/> <math>C_6H_4I_2</math>: d449<br/> <math>C_6H_4N_2</math>: a267, c328, c329, c330<br/> <math>C_6H_4N_2O_2</math>: b43<br/> <math>C_6H_4N_2O_4</math>: d711<br/> <math>C_6H_4N_2O_5</math>: d720<br/> <math>C_6H_4N_4O_6</math>: t402<br/> <math>C_6H_4O_2</math>: b58<br/> <math>C_6H_5BO_2</math>: c22<br/> <math>C_6H_5Br</math>: b262<br/> <math>C_6H_5BrO</math>: b392, b393, b394<br/> <math>C_6H_5BrS</math>: b428<br/> <math>C_6H_5Cl</math>: c47<br/> <math>C_6H_5ClHg</math>: p129<br/> <math>C_6H_5ClN_2O_2</math>: c188, c189, c190, c191<br/> <math>C_6H_5ClN_3O_4</math>: c113<br/> <math>C_6H_5ClO</math>: c208, c209, c210<br/> <math>C_6H_5ClO_2</math>: c102, c103, c244<br/> <math>C_6H_5ClO_2S</math>: b24<br/> <math>C_6H_5ClO_3S</math>: c49<br/> <math>C_6H_5ClS</math>: c252<br/> <math>C_6H_5Cl_2N</math>: d187, d188, d189, d190, d191, d192<br/> <math>C_6H_5Cl_2OP</math>: p140<br/> <math>C_6H_5Cl_2O_2P</math>: p100<br/> <math>C_6H_5Cl_2P</math>: d260<br/> <math>C_6H_5Cl_3Si</math>: p159<br/> <math>C_6H_5F</math>: f11<br/> <math>C_6H_5FN_2O_2</math>: f22<br/> <math>C_6H_5FO</math>: f28<br/> <math>C_6H_5FO_2S</math>: b25<br/> <math>C_6H_5I</math>: b28, i23<br/> <math>C_6H_5NO</math>: n77, p261, p262, p263<br/> <math>C_6H_5NOS</math>: t148<br/> <math>C_6H_5NO_2</math>: n30, n82, p265, p266, p267<br/> <math>C_6H_5NO_3</math>: h182, n59, n60<br/> <math>C_6H_5NO_4</math>: c288<br/> <math>C_6H_5N_3</math>: b61<br/> <math>C_6H_5N_3O</math>: h104<br/> <math>C_6H_5N_3O_4</math>: d710<br/> <math>C_6H_6</math>: b8<br/> <math>^{13}C_6H_6</math>: b10<br/> <math>C_6H_6AsNO_6</math>: h162<br/> <math>C_6H_6BrN</math>: b256, b257, b258<br/> <math>C_6H_6ClN</math>: c38, c39, c40<br/> <math>C_6H_6ClNO</math>: a147, c162<br/> <math>C_6H_6ClNO_2S</math>: c48<br/> <math>C_6H_6Cl_6</math>: h24<br/> <math>C_6H_6FN</math>: f7, f8<br/> <math>C_6H_6F_9O_3P</math>: t447<br/> <math>C_6H_6HgO</math>: p130 </p> |
| <p> <math>C_6</math> </p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| <p> <math>C_6BrD_5</math>: b263<br/> <math>C_6BrF_5</math>: b386<br/> <math>C_6Cl_4O_2</math>: t34, t35<br/> <math>C_6Cl_5NO_2</math>: p8 </p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                       |                                                                                                                   |                                                                                                                                                                                |
|-----------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| C <sub>6</sub> H <sub>6</sub> IN: i22                                                                                 | C <sub>6</sub> H <sub>9</sub> BrO <sub>3</sub> : b285                                                             | C <sub>6</sub> H <sub>12</sub> F <sub>3</sub> NOSi: m457                                                                                                                       |
| C <sub>6</sub> H <sub>6</sub> NO <sub>6</sub> : n20                                                                   | C <sub>6</sub> H <sub>9</sub> ClO <sub>3</sub> : e106, e107                                                       | C <sub>6</sub> H <sub>12</sub> NO <sub>3</sub> P: d294                                                                                                                         |
| C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O: e49, p259, p260, p264                                                 | C <sub>6</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> : b605                                                | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> : d61, d325, t279                                                                                                                |
| C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> : n23, n24, n25                                           | C <sub>6</sub> H <sub>9</sub> NO: o62, v17                                                                        | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S: b183, t119                                                                                                                    |
| C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> : a238, a239, a240, m94                                   | C <sub>6</sub> H <sub>9</sub> NOS: m433                                                                           | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S <sub>4</sub> : t120                                                                                                            |
| C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub> : d721, n53                                               | C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> : b540                                                              | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> Si: t396                                                                                                                         |
| C <sub>6</sub> H <sub>6</sub> O: p65                                                                                  | C <sub>6</sub> H <sub>9</sub> NO <sub>3</sub> : m78, n49                                                          | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> Zn: d601                                                                                                                         |
| C <sub>6</sub> H <sub>6</sub> OS: a57, m443                                                                           | C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> : a156                                                               | C <sub>6</sub> H <sub>12</sub> N <sub>4</sub> : h49                                                                                                                            |
| C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> : a44, c21, d428, d429, d430, h86, m258, r2                              | C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> : a157, c317, h83                                     | C <sub>6</sub> H <sub>12</sub> O: a96, b609, c365, d572, e11, e98, h51, h70, h71, h76, i78, m367, m430                                                                         |
| C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> S: b21, t152                                                             | C <sub>6</sub> H <sub>10</sub> : c368, d566, h39, h82, m356                                                       | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> : b465, b501, b502, b503, c359, d576, d577, e99, e100, e192, e209, e213, h64, h150, i63, m235, m312, m362, m363, m456, p244, t84 |
| C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> : b34, m259a, t317, t318                                                 | C <sub>6</sub> H <sub>10</sub> Br <sub>2</sub> : d89                                                              | C <sub>6</sub> H <sub>12</sub> O <sub>3</sub> : d525, e42, e179, e182, i116, p2, p237, t70                                                                                     |
| C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> S: b23                                                                   | C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> : e211, i114, p181                                                  | C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> : e149                                                                                                                           |
| C <sub>6</sub> H <sub>6</sub> O <sub>4</sub> : d529                                                                   | C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> : c361                                               | C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> Si: d27                                                                                                                          |
| C <sub>6</sub> H <sub>6</sub> O <sub>6</sub> : p206                                                                   | C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> : d338                                               | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> : f41, g1, g8, i19, m11, s6                                                                                                      |
| C <sub>6</sub> H <sub>6</sub> S: t156                                                                                 | C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub> : a14                                                | C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> : g6                                                                                                                             |
| C <sub>6</sub> H <sub>7</sub> AsO <sub>3</sub> : b12                                                                  | C <sub>6</sub> H <sub>10</sub> N <sub>4</sub> : p27                                                               | C <sub>6</sub> H <sub>12</sub> S: c364                                                                                                                                         |
| C <sub>6</sub> H <sub>7</sub> BO <sub>2</sub> : b13                                                                   | C <sub>6</sub> H <sub>10</sub> O: c366, c370, d31, d362, e12, h77, m224, m368, m370, m372                         | C <sub>6</sub> H <sub>13</sub> Br: b346                                                                                                                                        |
| C <sub>6</sub> H <sub>7</sub> ClN <sub>3</sub> : c216, c217                                                           | C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> : a91, c397, d422, e114, e119, e142, e199, h60, h69, h74, h75, m369 | C <sub>6</sub> H <sub>13</sub> BrO <sub>2</sub> : b317                                                                                                                         |
| C <sub>6</sub> H <sub>7</sub> N: a293, a294, m409, m410, m411                                                         | C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> : d501, e58, e143, h126, h177, m402, p214                           | C <sub>6</sub> H <sub>13</sub> Cl: c149                                                                                                                                        |
| C <sub>6</sub> H <sub>7</sub> NO: a252, a253, a254, h155, m113, p273, p274                                            | C <sub>6</sub> H <sub>10</sub> O <sub>4</sub> : d385, d634, d691, e22, e137, h54, m276, m303                      | C <sub>6</sub> H <sub>13</sub> ClO: c150                                                                                                                                       |
| C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub> : m414                                                                  | C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> : t146                                                              | C <sub>6</sub> H <sub>13</sub> ClO <sub>2</sub> : c96                                                                                                                          |
| C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub> S: b22                                                                  | C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> : d794, e136                                                        | C <sub>6</sub> H <sub>13</sub> ClO <sub>3</sub> : c124                                                                                                                         |
| C <sub>6</sub> H <sub>7</sub> NO <sub>3</sub> S: a115, a116, a117, s25                                                | C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> : d386                                                              | C <sub>6</sub> H <sub>13</sub> I: i36                                                                                                                                          |
| C <sub>6</sub> H <sub>7</sub> NS: a287                                                                                | C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> : d699, g7                                                          | C <sub>6</sub> H <sub>13</sub> N: c375, e202, h48, m383, m384, m385, m386                                                                                                      |
| C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub> : n65, n66, n67                                           | C <sub>6</sub> H <sub>10</sub> S: d34                                                                             | C <sub>6</sub> H <sub>13</sub> NO: d314, d637, e223, h133, h152                                                                                                                |
| C <sub>6</sub> H <sub>7</sub> O <sub>2</sub> P: p138                                                                  | C <sub>6</sub> H <sub>11</sub> Br: b311                                                                           | C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> : a182, a183, h127, i88, L5, L6, m233                                                                                           |
| C <sub>6</sub> H <sub>7</sub> O <sub>3</sub> P: p139                                                                  | C <sub>6</sub> H <sub>11</sub> BrO: b424                                                                          | C <sub>6</sub> H <sub>13</sub> NO <sub>4</sub> : b199                                                                                                                          |
| C <sub>6</sub> H <sub>8</sub> AsNO <sub>3</sub> : a113                                                                | C <sub>6</sub> H <sub>11</sub> BrO <sub>2</sub> : b279, b347, b529, e85, e86, e89                                 | C <sub>6</sub> H <sub>13</sub> NO <sub>5</sub> : t441                                                                                                                          |
| C <sub>6</sub> H <sub>8</sub> Br <sub>2</sub> O <sub>2</sub> : d107                                                   | C <sub>6</sub> H <sub>11</sub> BrO <sub>4</sub> : d346                                                            | C <sub>6</sub> H <sub>14</sub> : d567, d568, h52, m357, m358                                                                                                                   |
| C <sub>6</sub> H <sub>8</sub> Br <sub>3</sub> O: t205                                                                 | C <sub>6</sub> H <sub>11</sub> Cl: c91                                                                            | C <sub>6</sub> H <sub>14</sub> ClN: d328                                                                                                                                       |
| C <sub>6</sub> H <sub>8</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub> : a137                                   | C <sub>6</sub> H <sub>11</sub> ClO: h72                                                                           | C <sub>6</sub> H <sub>14</sub> Cl <sub>4</sub> OSi <sub>2</sub> : b175                                                                                                         |
| C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub> : m228                                                   | C <sub>6</sub> H <sub>11</sub> ClO <sub>2</sub> : b535, c82, e98                                                  | C <sub>6</sub> H <sub>14</sub> NO <sub>2</sub> : b213                                                                                                                          |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> : a218, a219, a220, a221, a222, a223, d284, m263, p104, p105, p106, p117 | C <sub>6</sub> H <sub>11</sub> I: i28                                                                             | C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> : a214, c354, d43, d44, d671, e245                                                                                               |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O: a204, o69                                                             | C <sub>6</sub> H <sub>11</sub> N: d30, h61, m361                                                                  | C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O: a172, h129                                                                                                                    |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S: b26, s24                                               | C <sub>6</sub> H <sub>11</sub> NO: c367, e260, f40, m388, o61, t379                                               | C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> : L13                                                                                                             |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> : d561a                                                   | C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> : e66                                                              | C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> : a301                                                                                                            |
| C <sub>6</sub> H <sub>8</sub> O: c371, d609, d620, h38                                                                | C <sub>6</sub> H <sub>12</sub> : c347, d572a, d573, d574, e95a, h73, m222                                         | C <sub>6</sub> H <sub>14</sub> O: b554, d476, d570, d570a, d571, d786, e95, h66, h67, h68, m364, m365, m366                                                                    |
| C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> : b451, c360, h40, m223                                                  | C <sub>6</sub> H <sub>12</sub> Br <sub>2</sub> : d94, d106                                                        | C <sub>6</sub> H <sub>14</sub> OSi: a93                                                                                                                                        |
| C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> : a36, a311, d599, f47                                                   | C <sub>6</sub> H <sub>12</sub> ClNO: c133                                                                         |                                                                                                                                                                                |
| C <sub>6</sub> H <sub>8</sub> O <sub>4</sub> : d598, d608, d629, d630                                                 | C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> : d217, d219, d234                                                 |                                                                                                                                                                                |
| C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> : a302, g11, i61                                                         | C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> O: b166                                                            |                                                                                                                                                                                |
| C <sub>6</sub> H <sub>8</sub> O <sub>7</sub> : c289                                                                   | C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>2</sub> : b161, d169                                        |                                                                                                                                                                                |
| C <sub>6</sub> H <sub>9</sub> Br: b312                                                                                | C <sub>6</sub> H <sub>12</sub> Cl <sub>3</sub> O <sub>3</sub> P: t437                                             |                                                                                                                                                                                |
|                                                                                                                       | C <sub>6</sub> H <sub>12</sub> Cl <sub>3</sub> O <sub>4</sub> P: t436                                             |                                                                                                                                                                                |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> : b493, d303, d304,<br>d569, e138, e219, h55, h56,<br>h57, m82, m360, p220                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | C <sub>6</sub> H <sub>18</sub> O <sub>3</sub> Si <sub>3</sub> : h45<br>C <sub>6</sub> H <sub>19</sub> NOSi <sub>2</sub> : b233<br>C <sub>6</sub> H <sub>19</sub> NSi <sub>2</sub> : h46                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub> : n26, n27<br>C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub> S: s1<br>C <sub>7</sub> H <sub>5</sub> NO <sub>4</sub> : n35, n36, n37, p268,<br>p269, p270<br>C <sub>7</sub> H <sub>5</sub> NO <sub>5</sub> : h163<br>C <sub>7</sub> H <sub>5</sub> NS: b59, p125<br>C <sub>7</sub> H <sub>5</sub> NS <sub>2</sub> : m17, m19<br>C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> : a234, n34, n55<br>C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> S: a236<br>C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub> : t405<br>C <sub>7</sub> H <sub>6</sub> BrClO: b300<br>C <sub>7</sub> H <sub>6</sub> BrNO <sub>2</sub> : n44<br>C <sub>7</sub> H <sub>6</sub> BrNO <sub>3</sub> : h156<br>C <sub>7</sub> H <sub>6</sub> Br <sub>2</sub> : b271, d132<br>C <sub>7</sub> H <sub>6</sub> Br <sub>2</sub> O: d111<br>C <sub>7</sub> H <sub>6</sub> ClF: c143, c144, f16<br>C <sub>7</sub> H <sub>6</sub> ClNO: c46<br>C <sub>7</sub> H <sub>6</sub> ClNO <sub>2</sub> : a138, a139, c202,<br>c203, n45<br>C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub> : c69, c70, d273, d274,<br>d275, d276<br>C <sub>7</sub> H <sub>6</sub> F <sub>3</sub> N: a126, a127, a128,<br>t310<br>C <sub>7</sub> H <sub>6</sub> FNO <sub>2</sub> : f24<br>C <sub>7</sub> H <sub>6</sub> INO <sub>2</sub> : a199<br>C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> : a121, a122, a123, b39<br>C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> : n28, n29<br>C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub> : a233, d723, d724<br>C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub> : d715, d716<br>C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> S: a125<br>C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub> : t134<br>C <sub>7</sub> H <sub>6</sub> O: b3<br>C <sub>7</sub> H <sub>6</sub> OS: t139<br>C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> : b44, h94, h95, h96,<br>m251<br>C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> S: m18<br>C <sub>7</sub> H <sub>6</sub> O <sub>3</sub> : d427, f46, h99, h100,<br>h101<br>C <sub>7</sub> H <sub>6</sub> O <sub>4</sub> : d431, d432, d433,<br>d434<br>C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> : t319<br>C <sub>7</sub> H <sub>6</sub> O <sub>6</sub> S: s31<br>C <sub>7</sub> H <sub>7</sub> Br: b85, b429, b430,<br>b431<br>C <sub>7</sub> H <sub>7</sub> BrO: b259, b260, b270,<br>b357, b358, b359<br>C <sub>7</sub> H <sub>7</sub> BrS: b425<br>C <sub>7</sub> H <sub>7</sub> Cl: b90, c255, c256, c257<br>C <sub>7</sub> H <sub>7</sub> ClNNaO <sub>2</sub> S: c258<br>C <sub>7</sub> H <sub>7</sub> ClN <sub>4</sub> O <sub>2</sub> : c253<br>C <sub>7</sub> H <sub>7</sub> ClO: c66, c160, c176,<br>c177<br>C <sub>7</sub> H <sub>7</sub> ClO <sub>2</sub> S: t177<br>C <sub>7</sub> H <sub>7</sub> ClO <sub>3</sub> S: m56 |
| C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> S: d789<br>C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> : b204, b214, d305,<br>d779, e41, e183, h63, h176,<br>t321, t341<br>C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> : t280<br>C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S: d788<br>C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>2</sub> : b459<br>C <sub>6</sub> H <sub>14</sub> O <sub>6</sub> : d824, m10, s5<br>C <sub>6</sub> H <sub>14</sub> O <sub>6</sub> S <sub>2</sub> : b210<br>C <sub>6</sub> H <sub>14</sub> S: b557, h62<br>C <sub>6</sub> H <sub>14</sub> Si: a101<br>C <sub>6</sub> H <sub>15</sub> Al: t273<br>C <sub>6</sub> H <sub>15</sub> AlI: d322<br>C <sub>6</sub> H <sub>15</sub> AlO: d321<br>C <sub>6</sub> H <sub>15</sub> As: t276<br>C <sub>6</sub> H <sub>15</sub> B: t277<br>C <sub>6</sub> H <sub>15</sub> ClGe: c260<br>C <sub>6</sub> H <sub>15</sub> ClO <sub>3</sub> Si: c240<br>C <sub>6</sub> H <sub>15</sub> ClSi: b551, c261<br>C <sub>6</sub> H <sub>15</sub> Ga: t286<br>C <sub>6</sub> H <sub>15</sub> In: t288<br>C <sub>6</sub> H <sub>15</sub> N: d468, d575, d777,<br>e97, h81, m371, t274<br>C <sub>6</sub> H <sub>15</sub> NO: a184, a211, a212,<br>b513, b553, d327, d364,<br>i98<br>C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub> : d306, d540, e125<br>C <sub>6</sub> H <sub>15</sub> NO <sub>3</sub> : t266<br>C <sub>6</sub> H <sub>15</sub> N <sub>3</sub> : a174<br>C <sub>6</sub> H <sub>15</sub> O <sub>3</sub> B: t268<br>C <sub>6</sub> H <sub>15</sub> O <sub>3</sub> P: d480, t294<br>C <sub>6</sub> H <sub>15</sub> O <sub>3</sub> PS: t298<br>C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P: t292<br>C <sub>6</sub> H <sub>15</sub> P: t293<br>C <sub>6</sub> H <sub>15</sub> Sb: t275<br>C <sub>6</sub> H <sub>16</sub> Br <sub>2</sub> OSi <sub>2</sub> : b149<br>C <sub>6</sub> H <sub>16</sub> Cl <sub>2</sub> OSi <sub>2</sub> : b167<br>C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> : d367, h53, m359,<br>t108<br>C <sub>6</sub> H <sub>16</sub> OSi: p221<br>C <sub>6</sub> H <sub>16</sub> O <sub>2</sub> Si: d301<br>C <sub>6</sub> H <sub>16</sub> O <sub>3</sub> SSi: m24<br>C <sub>6</sub> H <sub>16</sub> O <sub>3</sub> Si: t269, t342<br>C <sub>6</sub> H <sub>16</sub> Si: t297<br>C <sub>6</sub> H <sub>17</sub> NO <sub>3</sub> Si: a274, t344<br>C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> : i9<br>C <sub>6</sub> H <sub>18</sub> ClN <sub>3</sub> Si: c268a<br>C <sub>6</sub> H <sub>18</sub> N <sub>2</sub> Si: b179<br>C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> OP: h50<br>C <sub>6</sub> H <sub>18</sub> N <sub>4</sub> : t285, t434<br>C <sub>6</sub> H <sub>18</sub> OSi <sub>2</sub> : h47 | C <sub>7</sub> H <sub>3</sub> BrClF <sub>3</sub> : b297<br>C <sub>7</sub> H <sub>3</sub> BrF <sub>3</sub> NO: b380<br>C <sub>7</sub> H <sub>3</sub> ClF <sub>3</sub> NO <sub>2</sub> : c199, c200<br>C <sub>7</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>5</sub> : d714<br>C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> F <sub>3</sub> : d206, d207<br>C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> NO: d259<br>C <sub>7</sub> H <sub>3</sub> Cl <sub>3</sub> O: d208, d209<br>C <sub>7</sub> H <sub>4</sub> BrF <sub>3</sub> : b268, b269<br>C <sub>7</sub> H <sub>4</sub> Br <sub>2</sub> O: t15<br>C <sub>7</sub> H <sub>4</sub> ClFO: f14, f15<br>C <sub>7</sub> H <sub>4</sub> ClF <sub>3</sub> : c60, c61, c62<br>C <sub>7</sub> H <sub>4</sub> ClN: c54, c55<br>C <sub>7</sub> H <sub>4</sub> ClNO: c219, c220<br>C <sub>7</sub> H <sub>4</sub> ClNO <sub>3</sub> : n39, n40<br>C <sub>7</sub> H <sub>4</sub> ClNO <sub>4</sub> : c195, c196, c197<br>C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> O: c64, c65, d194,<br>d195<br>C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub> : d202, d203, d204<br>C <sub>7</sub> H <sub>4</sub> Cl <sub>3</sub> F: t238<br>C <sub>7</sub> H <sub>4</sub> Cl <sub>4</sub> : c58, c59<br>C <sub>7</sub> H <sub>4</sub> F <sub>3</sub> NO <sub>2</sub> : n86, n87<br>C <sub>7</sub> H <sub>4</sub> I <sub>2</sub> O <sub>3</sub> : h113<br>C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O: n38<br>C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>6</sub> : d713<br>C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>7</sub> : d722, h114<br>C <sub>7</sub> H <sub>4</sub> O <sub>3</sub> S: h105<br>C <sub>7</sub> H <sub>4</sub> O <sub>4</sub> S: s27<br>C <sub>7</sub> H <sub>5</sub> BrO: b65<br>C <sub>7</sub> H <sub>5</sub> BrO <sub>2</sub> : b266, b265<br>C <sub>7</sub> H <sub>5</sub> BrO <sub>3</sub> : b419<br>C <sub>7</sub> H <sub>5</sub> ClF <sub>3</sub> N: a142, a143<br>C <sub>7</sub> H <sub>5</sub> ClO: b66, c43, c44, c45<br>C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub> : c51, c52, c53, p99<br>C <sub>7</sub> H <sub>5</sub> ClO <sub>3</sub> : c207, c245, c246<br>C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> F: c139<br>C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NO: d196, d197<br>C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub> : t251, t252, t253, t254<br>C <sub>7</sub> H <sub>5</sub> FO: b68, f9, f10<br>C <sub>7</sub> H <sub>5</sub> FO <sub>2</sub> : f12, f13<br>C <sub>7</sub> H <sub>5</sub> F <sub>3</sub> : t311<br>C <sub>7</sub> H <sub>5</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub> : a237<br>C <sub>7</sub> H <sub>5</sub> F <sub>3</sub> O: t304<br>C <sub>7</sub> H <sub>5</sub> F <sub>4</sub> N: a179<br>C <sub>7</sub> H <sub>5</sub> IO <sub>2</sub> : i25<br>C <sub>7</sub> H <sub>5</sub> IO <sub>3</sub> : i51<br>C <sub>7</sub> H <sub>5</sub> I <sub>2</sub> NO <sub>2</sub> : a154<br>C <sub>7</sub> H <sub>5</sub> N: b51<br>C <sub>7</sub> H <sub>5</sub> NO: b62, p124 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p> <math>C_7H_7ClSi</math>: c73<br/> <math>C_7H_7Cl_3Si</math>: b128<br/> <math>C_7H_7F</math>: f27, f28, f29<br/> <math>C_7H_7FO</math>: f19, f20<br/> <math>C_7H_7FO_2S</math>: t178<br/> <math>C_7H_7I</math>: i53, i54, i55<br/> <math>C_7H_7N</math>: v15, v16<br/> <math>C_7H_7NO</math>: a53, a54, a55, b4, f35<br/> <math>C_7H_7NO_2</math>: a118, a119, a120, h97, h98, m412, m413, n83, n84, n85<br/> <math>C_7H_7NO_3</math>: a280, a281, m92, m339, m340, n41, n42, n43<br/> <math>C_7H_7NO_4S</math>: c17<br/> <math>C_7H_7N_3</math>: a197, a198<br/> <math>C_7H_8</math>: b134, c344, t166<br/> <math>C_7H_8BrN</math>: b360<br/> <math>C_7H_8ClN</math>: c37, c67, c68, c163, c164, c165, c166, c167<br/> <math>C_7H_8ClNO</math>: c158, c159<br/> <math>C_7H_8ClNO_2</math>: c19<br/> <math>C_7H_8ClNO_2S</math>: c248<br/> <math>C_7H_8Cl_2Si</math>: d239<br/> <math>C_7H_8N_2</math>: h102<br/> <math>C_7H_8N_2O</math>: a112, b71, p167<br/> <math>C_7H_8N_2O_2</math>: d40, h149, h170, m326, m327, m328, m329, m330, m415<br/> <math>C_8H_8N_2O_3</math>: m89, m90, m91<br/> <math>C_7H_8N_2S</math>: p158<br/> <math>C_7H_8N_4O_2</math>: t133<br/> <math>C_7H_8O</math>: b78, c303, c304, c305, m55<br/> <math>C_7H_8O_2</math>: d438, h106, m97, m98, m99, m280<br/> <math>C_7H_8O_2S</math>: t172<br/> <math>C_7H_8O_3</math>: e155, f49, m314<br/> <math>C_7H_8O_3S</math>: m139, t176<br/> <math>C_7H_8S</math>: b106, m379, t142<br/> <math>C_7H_9BrO_2</math>: e84<br/> <math>C_7H_9N</math>: b79, d685, d686, d687, d688, d689, e256, e257, e258, m134, t180, t181, t182<br/> <math>C_7H_9NO</math>: a213, b101, h132, m48, m49, m50<br/> <math>C_7H_9NO_2</math>: d524<br/> <math>C_7H_9NO_2S</math>: t173, t174<br/> <math>C_7H_9NO_3S</math>: a205, a206, a288<br/> <math>C_7H_9NS</math>: m436<br/> <math>C_7H_{10}</math>: b135<br/> <math>C_7H_{10}ClN_3O</math>: g4<br/> <math>C_7H_{10}N_2</math>: a177, a178, d59, d60, d287, d551, t167, t168, t169, t170 </p> | <p> <math>C_7H_{10}N_2O</math>: o66<br/> <math>C_7H_{10}N_2O_2</math>: e212, m242<br/> <math>C_7H_{10}N_2O_2S</math>: t175<br/> <math>C_7H_{10}O</math>: d294, m67, n108, t67<br/> <math>C_7H_{10}O_2</math>: a40, c402<br/> <math>C_7H_{10}O_3</math>: e17, e144, m354, t367<br/> <math>C_7H_{10}O_4</math>: d29, d596, p208<br/> <math>C_7H_{10}O_5</math>: d528<br/> <math>C_7H_{11}Br</math>: b383<br/> <math>C_7H_{11}BrO_4</math>: d346<br/> <math>C_7H_{11}ClO</math>: c351<br/> <math>C_7H_{11}N</math>: c350<br/> <math>C_7H_{11}NO</math>: c381, h112<br/> <math>C_7H_{11}NO_2</math>: a52, b539<br/> <math>C_7H_{11}NO_3</math>: m83<br/> <math>C_7H_{11}NO_5</math>: a45<br/> <math>C_7H_{11}NS</math>: c382<br/> <math>C_7H_{12}</math>: c345, h20, m215, m216, n107<br/> <math>C_7H_{12}N_2O</math>: m464<br/> <math>C_7H_{12}O</math>: b506, c348, c352, c369, m212, m213, m214<br/> <math>C_7H_{12}O_2</math>: a80, b507a, b508, c353, d420, e126, i65<br/> <math>C_7H_{12}O_3</math>: e43, e201, e226, h178, t73<br/> <math>C_7H_{12}O_4</math>: d378, d379, d636, d656, h7, m76, m277, t125<br/> <math>C_7H_{12}O_6Si</math>: m448<br/> <math>C_7H_{13}Br</math>: b310, b367<br/> <math>C_7H_{13}BrO_2</math>: b390, e92<br/> <math>C_7H_{13}ClO</math>: h17<br/> <math>C_7H_{13}N</math>: a245<br/> <math>C_7H_{13}NO</math>: a307, b507, c380<br/> <math>C_7H_{13}NO_2</math>: d541<br/> <math>C_7H_{13}NO_3</math>: d418<br/> <math>C_7H_{14}</math>: c341, e118a, h18, h18a, h18b, m202<br/> <math>C_7H_{14}ClN</math>: c134<br/> <math>C_7H_{14}N_2</math>: d475<br/> <math>C_7H_{14}N_2O</math>: a272<br/> <math>C_7H_{14}N_2O_2</math>: e246<br/> <math>C_7H_{14}O</math>: c342, c384, d655, d658, h3, h14, h15, h16, m205, m206, m207, m208, m209, m210, m211, m271<br/> <math>C_7H_{14}O_2</math>: b559, b593, b594, d312, e128, e207, e208, e239, h9, i74, i91, i106, m270, p53, p228<br/> <math>C_7H_{14}O_2S</math>: b569<br/> <math>C_7H_{14}O_3</math>: b567, e130, e151<br/> <math>C_7H_{14}O_6</math>: m262 </p> | <p> <math>C_7H_{15}Br</math>: b343, b344<br/> <math>C_7H_{15}Cl</math>: c147<br/> <math>C_7H_{15}ClO_2</math>: c97<br/> <math>C_7H_{15}I</math>: i34<br/> <math>C_7H_{15}N</math>: c362, d672, e247, e248, m218, m219, m220<br/> <math>C_7H_{15}NO</math>: e186, h131, h134, m387, p182, p183<br/> <math>C_7H_{15}NO_2</math>: p286<br/> <math>C_7H_{15}NO_3</math>: m467<br/> <math>C_7H_{15}O_5P</math>: t296<br/> <math>C_7H_{16}</math>: d654, e238, h6, t361<br/> <math>C_7H_{16}BrNO_2</math>: a38<br/> <math>C_7H_{16}ClNO_2</math>: a39<br/> <math>C_7H_{16}N_2</math>: a210, a271, m308, t392<br/> <math>C_7H_{16}N_2S</math>: d482<br/> <math>C_7H_{16}O</math>: d657, h10, h11, h12, t362<br/> <math>C_7H_{16}O_2</math>: b498, b499, d311, d393, m405<br/> <math>C_7H_{16}O_2Si</math>: d310<br/> <math>C_7H_{16}O_3</math>: d784, t290<br/> <math>C_7H_{16}O_4</math>: t92, t284<br/> <math>C_7H_{16}S</math>: h8<br/> <math>C_7H_{17}N</math>: h19, m272<br/> <math>C_7H_{17}NO</math>: b500, d332, d333<br/> <math>C_7H_{17}NO_2</math>: b515, d331<br/> <math>C_7H_{17}NO_5</math>: m261<br/> <math>C_7H_{18}N_2</math>: d334, d392, t116<br/> <math>C_7H_{18}N_2O</math>: b180<br/> <math>C_7H_{18}N_2O_2</math>: a270<br/> <math>C_7H_{18}N_2O_4Si</math>: t348<br/> <math>C_7H_{18}O_2Si</math>: b607<br/> <math>C_7H_{18}O_3Si</math>: b606, i77, m451<br/> <math>C_7H_{19}NOSi_2</math>: b232<br/> <math>C_7H_{19}NSi</math>: d404<br/> <math>C_7H_{19}N_3</math>: d52<br/> <math>C_7H_{20}N_2OSi_2</math>: b236<br/> <math>C_7H_{22}O_4Si_3</math>: h5 </p> |
| $C_8$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| <p> <math>C_8Br_4O_3</math>: t17<br/> <math>C_8Cl_4O_3</math>: t40<br/> <math>C_8D_{10}</math>: e73<br/> <math>C_8F_{18}O_2S</math>: p59<br/> <math>C_8HCl_4NO_2</math>: t39<br/> <math>C_8H_3NO_5</math>: n72<br/> <math>C_8H_4BrNO_2</math>: b348<br/> <math>C_8H_4Cl_2O_2</math>: b15, b16, p172<br/> <math>C_8H_4Cl_2O_4</math>: d261<br/> <math>C_8H_4Cl_6</math>: b225<br/> <math>C_8H_4F_6</math>: b229<br/> <math>C_8H_4N_2</math>: d282, d283 </p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |



**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                     |                                                                         |                                                                      |
|---------------------------------------------------------------------|-------------------------------------------------------------------------|----------------------------------------------------------------------|
| C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> : p107  | C <sub>8</sub> H <sub>8</sub> Br <sub>2</sub> : d98, d134, d135         | C <sub>8</sub> H <sub>10</sub> O <sub>3</sub> S: e75, m447           |
| C <sub>8</sub> H <sub>4</sub> O <sub>3</sub> : p169                 | C <sub>8</sub> H <sub>8</sub> ClNO: c25, c26, c26a                      | C <sub>8</sub> H <sub>10</sub> O <sub>4</sub> : d668, d669, d670     |
| C <sub>8</sub> H <sub>5</sub> BrN: b272                             | C <sub>8</sub> H <sub>8</sub> ClNO <sub>3</sub> : a146                  | C <sub>8</sub> H <sub>10</sub> O <sub>8</sub> : b469                 |
| C <sub>8</sub> H <sub>5</sub> ClO <sub>2</sub> : c224               | C <sub>8</sub> H <sub>8</sub> ClNO <sub>3</sub> S: a10                  | C <sub>8</sub> H <sub>10</sub> S: b110                               |
| C <sub>8</sub> H <sub>5</sub> Cl <sub>3</sub> O: t223               | C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> : d277, d278, d279        | C <sub>8</sub> H <sub>11</sub> N: b108, d553, d554,                  |
| C <sub>8</sub> H <sub>5</sub> Cl <sub>3</sub> O <sub>3</sub> : t246 | C <sub>8</sub> H <sub>8</sub> HgO: p128                                 | d555, d556, d557, d558,                                              |
| C <sub>8</sub> H <sub>5</sub> D <sub>3</sub> O: a32                 | C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> : a255, m140               | d559, e68, e69, e70, e220,                                           |
| C <sub>8</sub> H <sub>5</sub> F <sub>3</sub> O <sub>2</sub> S: t132 | C <sub>8</sub> H <sub>8</sub> O: a31, e9, m138, p77, s12                | i130, m151, m152, p112,                                              |
| C <sub>8</sub> H <sub>5</sub> F <sub>6</sub> N: b228                | C <sub>8</sub> H <sub>8</sub> OS: m437                                  | t393                                                                 |
| C <sub>8</sub> H <sub>5</sub> NO: b67                               | C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> : b41, b99, h91, h92,      | C <sub>8</sub> H <sub>11</sub> NO: a173, a251, a256,                 |
| C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub> : i17, p171           | h93, m51, m52, m53, m141,                                               | a257, a295, d544, e32, h122,                                         |
| C <sub>8</sub> H <sub>5</sub> NO <sub>3</sub> : h171, i60           | m142, m143, m144, p80,                                                  | m62, m80, m81, p101, p275,                                           |
| C <sub>8</sub> H <sub>5</sub> NO <sub>6</sub> : n31, n32, n70, n71  | p81                                                                     | p276                                                                 |
| C <sub>8</sub> H <sub>6</sub> : p84                                 | C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> S: p156, t157              | C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub> : d488, d489, d490    |
| C <sub>8</sub> H <sub>5</sub> BrClO: b286                           | C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> : d425, h142, h165, m8,    | C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub> S: m446               |
| C <sub>8</sub> H <sub>6</sub> BrN: b397                             | m57, m58, m59, m281,                                                    | C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub> : e150                |
| C <sub>8</sub> H <sub>6</sub> Br <sub>2</sub> O: d78                | m424, p68, r4, t81                                                      | C <sub>8</sub> H <sub>12</sub> : c387, c388, v9                      |
| C <sub>8</sub> H <sub>6</sub> Br <sub>4</sub> : t18, t19, t20       | C <sub>8</sub> H <sub>8</sub> O <sub>4</sub> : d25, h143                | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> : d288, d665, t117, x9 |
| C <sub>8</sub> H <sub>6</sub> ClN: c71, c72, c215                   | C <sub>8</sub> H <sub>8</sub> O <sub>4</sub> S: a33                     | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> : d461  |
| C <sub>8</sub> H <sub>6</sub> ClNO <sub>3</sub> : c187              | C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> : m454                     | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> : d339  |
| C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O: c168, d185         | C <sub>8</sub> H <sub>9</sub> Br: b334a, b335, b443,                    | C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> : a313                 |
| C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub> : d256 | b444, b445, b446                                                        | C <sub>8</sub> H <sub>12</sub> O: e278                               |
| C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> : q4                   | C <sub>8</sub> H <sub>9</sub> BrO: b321, b338, b361                     | C <sub>8</sub> H <sub>12</sub> O <sub>2</sub> : d589, e262, n109     |
| C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O: q5                  | C <sub>8</sub> H <sub>9</sub> BrO <sub>2</sub> : b318                   | C <sub>8</sub> H <sub>12</sub> O <sub>3</sub> : e135, t74            |
| C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> : n64   | C <sub>8</sub> H <sub>9</sub> Cl: c127, c128, c269,                     | C <sub>8</sub> H <sub>12</sub> O <sub>4</sub> : c355, d28, d370,     |
| C <sub>8</sub> H <sub>6</sub> O: b42                                | c270, c271, c272, c273                                                  | d377, m36                                                            |
| C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> : b14, p170, t6        | C <sub>8</sub> H <sub>9</sub> ClO: c108, c218                           | C <sub>8</sub> H <sub>12</sub> O <sub>5</sub> : d530                 |
| C <sub>8</sub> H <sub>6</sub> O <sub>3</sub> : b69, f37, m250       | C <sub>8</sub> H <sub>9</sub> ClO <sub>2</sub> : c104                   | C <sub>8</sub> H <sub>12</sub> O <sub>6</sub> Si: t194               |
| C <sub>8</sub> H <sub>6</sub> O <sub>4</sub> : b17, b18, p168       | C <sub>8</sub> H <sub>9</sub> N: b104, i18                              | C <sub>8</sub> H <sub>13</sub> N: e238                               |
| C <sub>8</sub> H <sub>6</sub> S: b60                                | C <sub>8</sub> H <sub>9</sub> NO: a18, a105, a106,                      | C <sub>8</sub> H <sub>13</sub> NO <sub>4</sub> : m342                |
| C <sub>8</sub> H <sub>7</sub> Br: b420                              | a107, b98, m256                                                         | C <sub>8</sub> H <sub>14</sub> : c393, o19, o49, v8                  |
| C <sub>8</sub> H <sub>7</sub> BrO: b251, b253                       | C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> : a15, a16, a17, a207,    | C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> : p185, p281           |
| C <sub>8</sub> H <sub>7</sub> BrO <sub>2</sub> : b356, b396         | a208, b89, d638, d639,                                                  | C <sub>8</sub> H <sub>14</sub> NO <sub>4</sub> : d472                |
| C <sub>8</sub> H <sub>7</sub> BrO <sub>3</sub> : b355               | d640, d641, e226, e259,                                                 | C <sub>8</sub> H <sub>14</sub> O: b576, c392, d592,                  |
| C <sub>8</sub> H <sub>7</sub> ClO: c31, c32, c33, p83,              | m54, m129, p114, t77                                                    | d621, m217, m269, o50                                                |
| t187, t188, t189                                                    | C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub> : a202, h167, h168,       | C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> : b464, b570, c373,    |
| C <sub>8</sub> H <sub>7</sub> ClO <sub>5</sub> : b92                | m95                                                                     | c374, c405, d620, h78, i71,                                          |
| C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub> : b91, c214, m60,    | C <sub>8</sub> H <sub>9</sub> NO <sub>4</sub> : d511                    | m203, n31                                                            |
| m191, m192, p69                                                     | C <sub>8</sub> H <sub>9</sub> NO <sub>4</sub> S: m133                   | C <sub>8</sub> H <sub>14</sub> O <sub>3</sub> : b505, b615, e45,     |
| C <sub>8</sub> H <sub>7</sub> ClO <sub>3</sub> : c161, c211         | C <sub>8</sub> H <sub>10</sub> : e74, x4, x5, x6                        | e101, i64, i82                                                       |
| C <sub>8</sub> H <sub>7</sub> FO: f6                                | C <sub>8</sub> H <sub>10</sub> ClN: c107                                | C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> : b197, b460, d381,    |
| C <sub>8</sub> H <sub>7</sub> N: i15, p82, t183, t184,              | C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O: d642                   | d396, d617, e139, e177, o25                                          |
| t185                                                                | C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> : m85      | C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> S: d703                |
| C <sub>8</sub> H <sub>7</sub> NO: m9, m147, t192                    | C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S: m343    | C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> S <sub>2</sub> : d793  |
| C <sub>8</sub> H <sub>7</sub> NS <sub>2</sub> : m438                | C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> : c1, d286 | C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> : d400, d401           |
| C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> : n21, n22            | C <sub>8</sub> H <sub>10</sub> O: b136, d659, d660,                     | C <sub>8</sub> H <sub>15</sub> BrO <sub>2</sub> : e88                |
| C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> S: t179               | d661, d662, d663, d664,                                                 | C <sub>8</sub> H <sub>15</sub> ClO: e163, o39                        |
| C <sub>8</sub> H <sub>7</sub> NO <sub>4</sub> : a114, m331, m332,   | e36, e240, e241, e242,                                                  | C <sub>8</sub> H <sub>15</sub> N: o28                                |
| m333, m334, m335, m336,                                             | m116, m117, m118, m149,                                                 | C <sub>8</sub> H <sub>15</sub> NO: p243                              |
| m337, n61, n62, n63                                                 | m150, p109, p110                                                        | C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub> : d543, e249, e250,   |
| C <sub>8</sub> H <sub>7</sub> NO <sub>5</sub> : m93                 | C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> : b19, d493, d494,        | p184                                                                 |
| C <sub>8</sub> H <sub>7</sub> NS: b126, m146                        | d495, e51, m61, m84, p72,                                               | C <sub>8</sub> H <sub>16</sub> : c389, d585, d586, d587,             |
| C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub> : a151  | p108                                                                    | d587a, d588, e117, o40, t384                                         |
| C <sub>8</sub> H <sub>8</sub> : s11                                 | C <sub>8</sub> H <sub>10</sub> O <sub>3</sub> : c308, c356, d512,       | C <sub>8</sub> H <sub>16</sub> Br <sub>2</sub> : d116                |
| C <sub>8</sub> H <sub>8</sub> BrNO: b248                            | h118, h145, m30, m234                                                   | C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S: h130 |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p> <math>C_8H_{16}O</math>: c378, c391, d500, d590, d591, e118, e158, m268, o36, o37, o38, o43<br/> <math>C_8H_{16}O_2</math>: b531, c357, c390, e160, e161, h79, i70, m266, o30, p239<br/> <math>C_8H_{16}O_3</math>: b497, e181<br/> <math>C_8H_{16}O_4</math>: c313, e37, t124<br/> <math>C_8H_{17}Br</math>: b385<br/> <math>C_8H_{17}Cl</math>: c204<br/> <math>C_8H_{17}Cl_3Si</math>: o48<br/> <math>C_8H_{17}I</math>: i44<br/> <math>C_8H_{17}N</math>: b597, c394, d593, d594<br/> <math>C_8H_{17}NO_3</math>: e173<br/> <math>C_8H_{17}O_3P</math>: t295<br/> <math>C_8H_{18}</math>: d616a, e158a e214, e215, o23, t100, t380, t381, t382<br/> <math>C_8H_{18}AlCl</math>: d455<br/> <math>C_8H_{18}ClNO_2</math>: a49<br/> <math>C_8H_{18}Cl_2Sn</math>: d177<br/> <math>C_8H_{18}F_3NOSi_2</math>: b235<br/> <math>C_8H_{18}N_2</math>: c349<br/> <math>C_8H_{18}N_2O_4S</math>: h130<br/> <math>C_8H_{18}N_2O_6S_2</math>: p179<br/> <math>C_8H_{18}O</math>: d148, d458, e162, m267, o32, o33, o34, o35, o66a<br/> <math>C_8H_{18}OSi_2</math>: d799<br/> <math>C_8H_{18}OSn</math>: d180<br/> <math>C_8H_{18}O_2</math>: b494, d159, d618, e159, o26, o27, t383<br/> <math>C_8H_{18}O_2S</math>: d173<br/> <math>C_8H_{18}O_3</math>: b186, b495, t289<br/> <math>C_8H_{18}O_3S</math>: d172<br/> <math>C_8H_{18}O_3Si</math>: t272<br/> <math>C_8H_{18}O_4</math>: b211, t282<br/> <math>C_8H_{18}O_4S</math>: d169<br/> <math>C_8H_{18}O_5</math>: t51<br/> <math>C_8H_{18}S</math>: d170, d171, o29<br/> <math>C_8H_{18}S_2</math>: b154, b155, d146, d147<br/> <math>C_8H_{18}Si_2</math>: b231<br/> <math>C_8H_{19}Al</math>: d456<br/> <math>C_8H_{19}N</math>: d139, d140, d457, d477, d619, e166, o44, t103<br/> <math>C_8H_{19}NO</math>: d413<br/> <math>C_8H_{19}NO_2</math>: b549, d299, d300<br/> <math>C_8H_{19}O_3P</math>: d164<br/> <math>C_8H_{20}BrN</math>: t49<br/> <math>C_8H_{20}ClN</math>: t50<br/> <math>C_8H_{20}Ge</math>: t58<br/> <math>C_8H_{20}N_2</math>: o24, t101, t102<br/> <math>C_8H_{20}N_2O_2S</math>: t61 </p> | <p> <math>C_8H_{20}O_3Si</math>: e270<br/> <math>C_8H_{20}O_4Si</math>: t48<br/> <math>C_8H_{20}O_4Ti</math>: t163<br/> <math>C_8H_{20}Pb</math>: t59<br/> <math>C_8H_{20}Si</math>: t60<br/> <math>C_8H_{20}Sn</math>: t63<br/> <math>C_8H_{21}NOSi_2</math>: b230<br/> <math>C_8H_{21}NO_2Si</math>: a269, d308<br/> <math>C_8H_{22}B</math>: b241<br/> <math>C_8H_{22}N_2O_3Si</math>: a166, t346<br/> <math>C_8H_{22}N_4</math>: b145<br/> <math>C_8H_{22}O_2Si_2</math>: b234<br/> <math>C_8H_{23}N_5</math>: t56<br/> <math>C_8H_{24}Cl_2O_3Si_4</math>: d250<br/> <math>C_8H_{24}O_2Si_3</math>: o22<br/> <math>C_8H_{24}O_4Si_4</math>: o21<br/> <math>C_8H_{35}N</math>: d728 </p> <hr/> <p style="text-align: center;"><math>C_9</math></p> <hr/> <p> <math>C_9H_2Cl_6O_3</math>: h28<br/> <math>C_9H_3Cl_3O_3</math>: b33<br/> <math>C_9H_4O_5</math>: b32<br/> <math>C_9H_5BrClNO</math>: b304<br/> <math>C_9H_5Br_2NO</math>: d108<br/> <math>C_9H_5ClINO</math>: c152<br/> <math>C_9H_5Cl_2N</math>: d270<br/> <math>C_9H_6BrN</math>: b418<br/> <math>C_9H_6ClNO</math>: c153<br/> <math>C_9H_6INO_2S</math>: h137<br/> <math>C_9H_6N_2O_2</math>: t171<br/> <math>C_9H_6O_2</math>: b55, c292<br/> <math>C_9H_6O_3</math>: h111<br/> <math>C_9H_6O_4</math>: i13<br/> <math>C_9H_6O_6</math>: b29, b30, b31<br/> <math>C_9H_7BrO</math>: b309<br/> <math>C_9H_7ClO</math>: c280<br/> <math>C_9H_7ClO_2</math>: c90<br/> <math>C_9H_7N</math>: i133, q3<br/> <math>C_9H_7NO</math>: h184<br/> <math>C_9H_7NO_3</math>: h151, m289<br/> <math>C_9H_7NO_4</math>: n50<br/> <math>C_9H_7NO_4S</math>: h185<br/> <math>C_9H_7N_3O_4S_2</math>: a242<br/> <math>C_9H_8</math>: i14<br/> <math>C_9H_8Cl_4O_3</math>: d258<br/> <math>C_9H_8N_2</math>: m423, p120<br/> <math>C_9H_8N_2O_6</math>: e129<br/> <math>C_9H_8O</math>: c278, i12<br/> <math>C_9H_8O_2</math>: c279, d417, v6<br/> <math>C_9H_8O_3</math>: h109<br/> <math>C_9H_8O_3S</math>: p247<br/> <math>C_9H_8O_4</math>: p127<br/> <math>C_9H_9BrO</math>: b412<br/> <math>C_9H_9BrO_2</math>: b86 </p> | <p> <math>C_9H_9Cl</math>: v7<br/> <math>C_9H_9ClO</math>: c234<br/> <math>C_9H_9ClO_2</math>: c213, d498<br/> <math>C_9H_9N</math>: d564, m287<br/> <math>C_9H_9NO</math>: m103, m104, p134<br/> <math>C_9H_9NO_2</math>: a9<br/> <math>C_9H_9NO_3</math>: a11, a12, b70<br/> <math>C_9H_9NO_4</math>: e227<br/> <math>C_9H_9N_3O</math>: a260<br/> <math>C_9H_9N_3O_2S_2</math>: t137<br/> <math>C_9H_9N_5</math>: d53<br/> <math>C_9H_{10}</math>: a78, i10, m425, m426<br/> <math>C_9H_{10}BrF_2</math>: d109<br/> <math>C_9H_{10}F_3NO_2</math>: m135<br/> <math>C_9H_{10}N</math>: a196, a197<br/> <math>C_9H_{10}N_2</math>: a296, p121<br/> <math>C_9H_{10}N_2O</math>: p151<br/> <math>C_9H_{10}N_2O_2</math>: p85<br/> <math>C_9H_{10}N_2O_3</math>: a129<br/> <math>C_9H_{10}O</math>: a94, a95, c282, e14, e72, i11, m124, p147, p148, p149, p209, p217<br/> <math>C_9H_{10}O_2</math>: b63, b76, d563, e33, e34, e76, h174, h175, m44, m45, m46, m309, m310, m311, m375, p103, p150, t190<br/> <math>C_9H_{10}O_3</math>: d491, d492, e37, e38, e46, e55, e178, e261, f52, m101, m283, m297, m304, m305, p74<br/> <math>C_9H_{10}O_4</math>: d496, d492, h135, m292<br/> <math>C_9H_{11}Br</math>: b350, b353, b399, b435, b436<br/> <math>C_9H_{11}BrO</math>: b413, p75<br/> <math>C_9H_{11}Cl</math>: c222<br/> <math>C_9H_{11}ClO_3S</math>: c135<br/> <math>C_9H_{11}N</math>: a77, c333, m288, t78, t86<br/> <math>C_9H_{11}NO</math>: d536, d562, m121, m374, m445<br/> <math>C_9H_{11}NO_2</math>: d537, d538, e35, e64, e65, i126, p86<br/> <math>C_9H_{11}NO_3</math>: t455<br/> <math>C_9H_{12}</math>: e190, i103, p225, t357, t358, t359, v13<br/> <math>C_9H_{12}N_2O_4</math>: a241<br/> <math>C_9H_{12}N_2O_6</math>: u18<br/> <math>C_9H_{12}N_2O_5S</math>: b111<br/> <math>C_9H_{12}O</math>: b98, d632, d633, i127, i128, i129, m373, p145, p146, p240, t385, t386, t387<br/> <math>C_9H_{12}O_2</math>: b115, c316, c358, e48, p73, p148, t365, t374 </p> |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                            |                                                                              |                                                                                                                                                    |
|--------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| C <sub>9</sub> H <sub>12</sub> O <sub>3</sub> : d499, m204, t332, t333, t334               | C <sub>9</sub> H <sub>20</sub> : d386a, d613a, e210a, n90, t370a             | C <sub>10</sub> H <sub>8</sub> O <sub>3</sub> S: n6, n7                                                                                            |
| C <sub>9</sub> H <sub>12</sub> O <sub>3</sub> S: e263                                      | C <sub>9</sub> H <sub>20</sub> Cl <sub>2</sub> Si: d238                      | C <sub>10</sub> H <sub>8</sub> O <sub>4</sub> : d443, d444                                                                                         |
| C <sub>9</sub> H <sub>12</sub> S: p144                                                     | C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> : a136, a290                   | C <sub>10</sub> H <sub>9</sub> N: a228, a229, m420, m421, m422, n17                                                                                |
| C <sub>9</sub> H <sub>13</sub> N: b595, d565, d706, e80, e203, e264 e265, e266, i101, t355 | C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> S: d136                        | C <sub>10</sub> H <sub>9</sub> NO: a51, a232                                                                                                       |
| C <sub>9</sub> H <sub>13</sub> NO: b80, m96, n110                                          | C <sub>9</sub> H <sub>20</sub> O: d615, n98, t371                            | C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub> : i16                                                                                               |
| C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub> : a258, b596                                | C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> : b556, n94                    | C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub> : h128                                                                                              |
| C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> : t191                                       | C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> Si: c377                       | C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub> S: a230                                                                                             |
| C <sub>9</sub> H <sub>14</sub> BrN: p162                                                   | C <sub>9</sub> H <sub>20</sub> O <sub>3</sub> : d783, t291                   | C <sub>10</sub> H <sub>9</sub> NO <sub>4</sub> S: a189, a190, a191, a192                                                                           |
| C <sub>9</sub> H <sub>14</sub> Br <sub>3</sub> N: p165                                     | C <sub>9</sub> H <sub>20</sub> O <sub>3</sub> Si: a99                        | C <sub>10</sub> H <sub>9</sub> NO <sub>6</sub> : d643                                                                                              |
| C <sub>9</sub> H <sub>14</sub> ClN: p163                                                   | C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> : t430                         | C <sub>10</sub> H <sub>10</sub> : d423                                                                                                             |
| C <sub>9</sub> H <sub>14</sub> IN: p164                                                    | C <sub>9</sub> H <sub>21</sub> Al: t428                                      | C <sub>10</sub> H <sub>10</sub> BrClO: b299                                                                                                        |
| C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> : n92, t388                                  | C <sub>9</sub> H <sub>21</sub> BO <sub>3</sub> : t427, t326                  | C <sub>10</sub> H <sub>10</sub> ClFO: c121                                                                                                         |
| C <sub>9</sub> H <sub>14</sub> O: d611, d613, i93, t364                                    | C <sub>9</sub> H <sub>21</sub> BO <sub>6</sub> : t445                        | C <sub>10</sub> H <sub>10</sub> ClNO <sub>2</sub> : c29                                                                                            |
| C <sub>9</sub> H <sub>14</sub> O <sub>2</sub> : m350                                       | C <sub>9</sub> H <sub>21</sub> ClO <sub>3</sub> Si: c239                     | C <sub>10</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>3</sub> : d257                                                                              |
| C <sub>9</sub> H <sub>14</sub> O <sub>2</sub> Si: d510                                     | C <sub>9</sub> H <sub>21</sub> N: n105, t429                                 | C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> : a279, n4, n5                                                                                      |
| C <sub>9</sub> H <sub>14</sub> O <sub>3</sub> : b215, t76                                  | C <sub>9</sub> H <sub>21</sub> NO <sub>2</sub> : d470, d778                  | C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O: m378                                                                                             |
| C <sub>9</sub> H <sub>14</sub> O <sub>3</sub> Si: p161                                     | C <sub>9</sub> H <sub>21</sub> NO <sub>3</sub> : t325                        | C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S: s21                                                                               |
| C <sub>9</sub> H <sub>14</sub> O <sub>5</sub> : d315, d382                                 | C <sub>9</sub> H <sub>21</sub> N <sub>3</sub> : t287                         | C <sub>10</sub> H <sub>10</sub> O: d363, m197, p94, p95                                                                                            |
| C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> : p200                                       | C <sub>9</sub> H <sub>21</sub> O <sub>3</sub> P: t329                        | C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> : b63, m66, m198, s2                                                                                |
| C <sub>9</sub> H <sub>14</sub> Si: p166                                                    | C <sub>9</sub> H <sub>22</sub> N <sub>2</sub> : d387, n91                    | C <sub>10</sub> H <sub>10</sub> O <sub>3</sub> : b72, m345                                                                                         |
| C <sub>9</sub> H <sub>15</sub> N: t195                                                     | C <sub>9</sub> H <sub>22</sub> O <sub>2</sub> : d780, d781                   | C <sub>10</sub> H <sub>10</sub> O <sub>4</sub> : d590, d591, d592, m125, p155, r3                                                                  |
| C <sub>9</sub> H <sub>15</sub> NO: c362                                                    | C <sub>9</sub> H <sub>22</sub> Si: t330                                      | C <sub>10</sub> H <sub>11</sub> BrO: b375                                                                                                          |
| C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> : t439                                       | C <sub>9</sub> H <sub>23</sub> N <sub>3</sub> : p26                          | C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub> : c212                                                                                            |
| C <sub>9</sub> H <sub>16</sub> : m348                                                      | C <sub>9</sub> H <sub>24</sub> N <sub>4</sub> : b147                         | C <sub>10</sub> H <sub>11</sub> ClO <sub>4</sub> : t336                                                                                            |
| C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> : d62                                        | C <sub>9</sub> H <sub>24</sub> O <sub>2</sub> Si <sub>3</sub> : m153         | C <sub>10</sub> H <sub>11</sub> IO <sub>4</sub> : i24                                                                                              |
| C <sub>9</sub> H <sub>16</sub> O: d612, n103                                               | C <sub>9</sub> H <sub>27</sub> BO <sub>3</sub> Si <sub>3</sub> : t449        | C <sub>10</sub> H <sub>11</sub> N: p98                                                                                                             |
| C <sub>9</sub> H <sub>16</sub> O <sub>2</sub> : b571, c363, h80, n97                       | C <sub>9</sub> H <sub>31</sub> ClO <sub>3</sub> Ti: c254                     | C <sub>10</sub> H <sub>11</sub> NO <sub>2</sub> : a24, d514                                                                                        |
| C <sub>9</sub> H <sub>16</sub> O <sub>3</sub> : b568, b582                                 |                                                                              | C <sub>10</sub> H <sub>11</sub> NO <sub>4</sub> : c8, d552a                                                                                        |
| C <sub>9</sub> H <sub>16</sub> O <sub>4</sub> : d368, d371, d478, d614, n93                | C <sub>10</sub> H <sub>2</sub> O <sub>6</sub> : b28                          | C <sub>10</sub> H <sub>11</sub> O <sub>2</sub> S: b94                                                                                              |
| C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> : d345                                       | C <sub>10</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub> : d243         | C <sub>10</sub> H <sub>12</sub> : d292, t80                                                                                                        |
| C <sub>9</sub> H <sub>17</sub> BrO <sub>2</sub> : e87                                      | C <sub>10</sub> H <sub>6</sub> Br <sub>2</sub> O: d113                       | C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> : a170, b81                                                                                         |
| C <sub>9</sub> H <sub>17</sub> Cl: c92                                                     | C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub> O: d242                       | C <sub>10</sub> H <sub>12</sub> O: a89, b77a, b619, e59, e279, i84, i102, m107, m403, p96                                                          |
| C <sub>9</sub> H <sub>17</sub> ClO: n102, t372                                             | C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> : b103                         | C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> : d419, e204, e205, e206, e243, h154, h166, m79, m102, m108, m109, m111, m148, p79, p97, p111, p226 |
| C <sub>9</sub> H <sub>17</sub> ClO <sub>2</sub> : e167                                     | C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub> : d719          | C <sub>10</sub> H <sub>12</sub> O <sub>3</sub> : d487, e47, e195, m306, p71, p102, p235                                                            |
| C <sub>9</sub> H <sub>17</sub> N: a83, n95                                                 | C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub> S: d64          | C <sub>10</sub> H <sub>12</sub> O <sub>4</sub> : d26a, d513, m231, m232, t331                                                                      |
| C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub> : e216, e217                                | C <sub>10</sub> H <sub>6</sub> O <sub>2</sub> : n11                          | C <sub>10</sub> H <sub>13</sub> O <sub>5</sub> : p245, t335                                                                                        |
| C <sub>9</sub> H <sub>18</sub> : i108, p229, t363                                          | C <sub>10</sub> H <sub>6</sub> O <sub>3</sub> : h161                         | C <sub>10</sub> H <sub>13</sub> Br: b280, b351                                                                                                     |
| C <sub>9</sub> H <sub>18</sub> NO: t115                                                    | C <sub>10</sub> H <sub>6</sub> O <sub>8</sub> : b27                          | C <sub>10</sub> H <sub>13</sub> BrO: b281                                                                                                          |
| C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O: d550                                      | C <sub>10</sub> H <sub>7</sub> Br: b376                                      | C <sub>10</sub> H <sub>13</sub> BrO <sub>2</sub> : b395                                                                                            |
| C <sub>9</sub> H <sub>18</sub> O: c385, d616, n99, n100, n101, n104, t370                  | C <sub>10</sub> H <sub>7</sub> BrO: b377, b378                               | C <sub>10</sub> H <sub>13</sub> Cl: b536, c178                                                                                                     |
| C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> : e156, m349, n96                            | C <sub>10</sub> H <sub>7</sub> Br <sub>2</sub> NO: d112                      | C <sub>10</sub> H <sub>13</sub> NO: d527, p131                                                                                                     |
| C <sub>9</sub> H <sub>18</sub> O <sub>3</sub> : d144                                       | C <sub>10</sub> H <sub>7</sub> Cl: c185, c186                                | C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> : m380                                                                                             |
| C <sub>9</sub> H <sub>18</sub> O <sub>4</sub> : d785                                       | C <sub>10</sub> H <sub>7</sub> ClO: c185, c186                               | C <sub>10</sub> H <sub>13</sub> NS <sub>2</sub> : b95                                                                                              |
| C <sub>9</sub> H <sub>19</sub> Br: b382                                                    | C <sub>10</sub> H <sub>7</sub> NO <sub>2</sub> : n57, n80, p126              |                                                                                                                                                    |
| C <sub>9</sub> H <sub>19</sub> BrO <sub>2</sub> : e90                                      | C <sub>10</sub> H <sub>7</sub> NO <sub>6</sub> S <sub>2</sub> : n81          |                                                                                                                                                    |
| C <sub>9</sub> H <sub>19</sub> I: i42                                                      | C <sub>10</sub> H <sub>8</sub> : a316, d1, n2                                |                                                                                                                                                    |
| C <sub>9</sub> H <sub>19</sub> NO: d151                                                    | C <sub>10</sub> H <sub>8</sub> BrNO <sub>2</sub> : b339                      |                                                                                                                                                    |
| C <sub>9</sub> H <sub>19</sub> NO <sub>3</sub> Si: t270                                    | C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> : d790                         |                                                                                                                                                    |
| C <sub>9</sub> H <sub>19</sub> N <sub>2</sub> S: d175                                      | C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> : b205, f53     |                                                                                                                                                    |
|                                                                                            | C <sub>10</sub> H <sub>8</sub> O: n9, n10                                    |                                                                                                                                                    |
|                                                                                            | C <sub>10</sub> H <sub>8</sub> O <sub>2</sub> : d439, d440, d441, d442, m199 |                                                                                                                                                    |
|                                                                                            | C <sub>10</sub> H <sub>8</sub> O <sub>3</sub> : h148                         |                                                                                                                                                    |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p> <math>C_{10}H_{13}N_5O_4</math>: a67<br/> <math>C_{10}H_{13}O_2S</math>: b94<br/> <math>C_{10}H_{14}</math>: b521, b522, b523, d340a, d341, d342, i67, i118, i119, i120, t97, t98, t99<br/> <math>C_{10}H_{14}ClN</math>: c130<br/> <math>C_{10}H_{14}NO_3PS</math>: p3<br/> <math>C_{10}H_{14}N_2</math>: n19, p141<br/> <math>C_{10}H_{14}N_2O</math>: d383<br/> <math>C_{10}H_{14}N_2O_4</math>: b206<br/> <math>C_{10}H_{14}N_4O_4</math>: d446<br/> <math>C_{10}H_{14}O</math>: c20, i104<br/> <math>C_{10}H_{14}O</math>: b585, b586, b587, b588, b591, c20, i104, i121, i122, i123, k2, m376, t162a, t260<br/> <math>C_{10}H_{14}O_2</math>: b534, d516, p78<br/> <math>C_{10}H_{14}O_3</math>: c7<br/> <math>C_{10}H_{14}O_4</math>: b461, e23, e140, m100, t337<br/> <math>C_{10}H_{14}O_3PS</math>: p3<br/> <math>C_{10}H_{15}BrO</math>: b284<br/> <math>C_{10}H_{15}N</math>: b516, b517, b518, b519, d336, d278, e2, e277, i105, i117, m377, p96<br/> <math>C_{10}H_{15}NO</math>: b490, c403, d330, e2, p219<br/> <math>C_{10}H_{15}NO_2</math>: d517<br/> <math>C_{10}H_{15}NO_4</math>: d309<br/> <math>C_{10}H_{16}</math>: a65, c2, d595, d648, d736, L7, L8, m467, p25, p175, p176, t10, t11, t259, t400a<br/> <math>C_{10}H_{16}ClN</math>: b131<br/> <math>C_{10}H_{16}Cl_2O_2</math>: d13<br/> <math>C_{10}H_{16}N_2</math>: d388<br/> <math>C_{10}H_{16}N_2O_4</math>: d35<br/> <math>C_{10}H_{16}N_2O_8</math>: e134<br/> <math>C_{10}H_{16}O</math>: c3, c4, c286, d416, d614, d645, L9, L10, p177, p250, t376<br/> <math>C_{10}H_{16}O_2</math>: c383, m344<br/> <math>C_{10}H_{16}O_4</math>: c4, d319<br/> <math>C_{10}H_{16}O_4S</math>: c5<br/> <math>C_{10}H_{16}O_5</math>: d317, d366<br/> <math>C_{10}H_{16}Si</math>: b132<br/> <math>C_{10}H_{17}N</math>: a64, p284<br/> <math>C_{10}H_{17}NO</math>: c386, m465<br/> <math>C_{10}H_{18}</math>: d2, d3<br/> <math>C_{10}H_{18}NO_2</math>: b514<br/> <math>C_{10}H_{18}N_2O_7</math>: h124<br/> <math>C_{10}H_{18}O</math>: b245, b545, b546, c277, d4, g2, i62, i132, L11, m13, t12, t13, t375 </p> | <p> <math>C_{10}H_{18}O_2</math>: c379, d17, d650<br/> <math>C_{10}H_{18}O_3</math>: d680, t77, t350, v1<br/> <math>C_{10}H_{18}O_4</math>: b185, d10, d58, d318, d394, d651, t283<br/> <math>C_{10}H_{18}O_6</math>: d481<br/> <math>C_{10}H_{18}S_2</math>: b154<br/> <math>C_{10}H_{19}ClO</math>: d21<br/> <math>C_{10}H_{19}N</math>: d13, d13a, t356<br/> <math>C_{10}H_{19}NO_2</math>: d329, e251<br/> <math>C_{10}H_{20}</math>: b541, b542, c335, d22<br/> <math>C_{10}H_{20}Br_2</math>: d91<br/> <math>C_{10}H_{20}Cl_2</math>: d216<br/> <math>C_{10}H_{20}N_2S_4</math>: t62<br/> <math>C_{10}H_{20}O</math>: b543, b544, c290, d7, d18, d19, d20, e7, e175, m12, m313<br/> <math>C_{10}H_{20}O_2</math>: d15, e164, e231, m177, o42<br/> <math>C_{10}H_{20}O_4</math>: b496, b530<br/> <math>C_{10}H_{20}O_5</math>: p46<br/> <math>C_{10}H_{20}O_5Si</math>: t347<br/> <math>C_{10}H_{21}Br</math>: b315<br/> <math>C_{10}H_{21}Cl</math>: c94<br/> <math>C_{10}H_{21}I</math>: i29<br/> <math>C_{10}H_{21}N</math>: d353<br/> <math>C_{10}H_{21}NO</math>: a226<br/> <math>C_{10}H_{21}NO_2</math>: e218<br/> <math>C_{10}H_{21}NO_4Si</math>: t271<br/> <math>C_{10}H_{22}</math>: d8<br/> <math>C_{10}H_{22}N_2</math>: d51<br/> <math>C_{10}H_{22}O</math>: d16, d646, d647, d738, t79<br/> <math>C_{10}H_{22}O_2</math>: d11, d12, d137<br/> <math>C_{10}H_{22}O_3</math>: d699, t433<br/> <math>C_{10}H_{22}O_4</math>: t432<br/> <math>C_{10}H_{22}O_5</math>: b212, p47, t55<br/> <math>C_{10}H_{22}O_7</math>: d735<br/> <math>C_{10}H_{23}N</math>: d23, d649, d737<br/> <math>C_{10}H_{23}NO</math>: d141<br/> <math>C_{10}H_{23}NO_2</math>: d313<br/> <math>C_{10}H_{24}N_2</math>: d9, t57, t111<br/> <math>C_{10}H_{24}N_2O_2</math>: d731<br/> <math>C_{10}H_{24}N_4</math>: b146, t89<br/> <math>C_{10}H_{24}O_3Si</math>: i76<br/> <math>C_{10}H_{28}N_6</math>: p23<br/> <math>C_{10}H_{30}O_3Si_4</math>: d6<br/> <math>C_{10}H_{30}O_5Si_5</math>: d5 </p> | <p> <math>C_{11}H_5Br</math>: b370<br/> <math>C_{11}H_9Cl</math>: c175<br/> <math>C_{11}H_9N</math>: p152<br/> <math>C_{11}H_{10}</math>: m318, m319<br/> <math>C_{11}H_{10}O</math>: m87, m88<br/> <math>C_{11}H_{12}ClF</math>: c140<br/> <math>C_{11}H_{12}N_2O</math>: a299<br/> <math>C_{11}H_{12}N_2O_2</math>: t454<br/> <math>C_{11}H_{12}O_2</math>: b107, c281, e112, m115<br/> <math>C_{11}H_{12}O_3</math>: b77, b200, e77, e145, e244<br/> <math>C_{11}H_{13}ClO</math>: b527<br/> <math>C_{11}H_{13}ClO_3</math>: c259<br/> <math>C_{11}H_{13}NO</math>: b124, d666<br/> <math>C_{11}H_{13}NO_4</math>: b580<br/> <math>C_{11}H_{13}N_3O</math>: a110<br/> <math>C_{11}H_{14}O</math>: p44, m114<br/> <math>C_{11}H_{14}O_2</math>: a84, b524, b526, d522, e52, e176, p113<br/> <math>C_{11}H_{14}O_3</math>: b491, b584, b590, e200<br/> <math>C_{11}H_{14}O_4</math>: e158<br/> <math>C_{11}H_{15}N</math>: p142<br/> <math>C_{11}H_{15}NO</math>: b121, d326<br/> <math>C_{11}H_{15}NO_2</math>: b512, d542, e127<br/> <math>C_{11}H_{16}</math>: b602, p24, p55<br/> <math>C_{11}H_{16}N_2</math>: b119<br/> <math>C_{11}H_{16}O</math>: b87, b573, b574, b575, d667, p57<br/> <math>C_{11}H_{16}O_4</math>: d800<br/> <math>C_{11}H_{17}N</math>: b538, d403<br/> <math>C_{11}H_{17}NO</math>: e267<br/> <math>C_{11}H_{17}NO_2</math>: b109, m416<br/> <math>C_{11}H_{17}O_3P</math>: d344<br/> <math>C_{11}H_{18}N_2O_3</math>: t366<br/> <math>C_{11}H_{18}O</math>: d372, n106<br/> <math>C_{11}H_{18}O_5</math>: d316<br/> <math>C_{11}H_{19}ClO</math>: u15<br/> <math>C_{11}H_{19}NO_2</math>: e168, o45<br/> <math>C_{11}H_{20}O</math>: u12<br/> <math>C_{11}H_{20}O_2</math>: e165, i89, u13<br/> <math>C_{11}H_{20}O_4</math>: d155, d347, d354, d373<br/> <math>C_{11}H_{21}BrO_2</math>: b442<br/> <math>C_{11}H_{21}N</math>: u3<br/> <math>C_{11}H_{21}O_2</math>: c287<br/> <math>C_{11}H_{22}</math>: u12a<br/> <math>C_{11}H_{22}N_2</math>: d776<br/> <math>C_{11}H_{22}O</math>: u1, u9, u10, u11, u14<br/> <math>C_{11}H_{22}O_2</math>: e171, e228, m69, m226, u4, u5, u6<br/> <math>C_{11}H_{23}Br</math>: b441<br/> <math>C_{11}H_{23}I</math>: i57<br/> <math>C_{11}H_{24}</math>: u2 </p> |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                             |                                                                               |                                                                       |
|-----------------------------------------------------------------------------|-------------------------------------------------------------------------------|-----------------------------------------------------------------------|
| C <sub>11</sub> H <sub>24</sub> O: u7, u8                                   | C <sub>12</sub> H <sub>11</sub> N <sub>3</sub> : p88                          | C <sub>12</sub> H <sub>22</sub> O <sub>11</sub> : L3, L4, m7, s20     |
| C <sub>11</sub> H <sub>24</sub> O <sub>6</sub> Si: t444                     | C <sub>12</sub> H <sub>11</sub> O <sub>3</sub> P: d763                        | C <sub>12</sub> H <sub>23</sub> N: d289                               |
| C <sub>11</sub> H <sub>25</sub> NO <sub>2</sub> : a292                      | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> : b140, d757, p137             | C <sub>12</sub> H <sub>23</sub> NO: a308, o47                         |
| C <sub>11</sub> H <sub>26</sub> N <sub>2</sub> : b555, d166                 | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O: o68                         | C <sub>12</sub> H <sub>24</sub> : d813                                |
| C <sub>11</sub> H <sub>26</sub> N <sub>2</sub> O <sub>6</sub> : b237        | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> : b40           | C <sub>12</sub> H <sub>24</sub> Cl <sub>2</sub> : d224                |
|                                                                             | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S: d47, d48     | C <sub>12</sub> H <sub>24</sub> O: c326, d817, e8, m459               |
|                                                                             | C <sub>12</sub> H <sub>12</sub> O: e50                                        | C <sub>12</sub> H <sub>24</sub> O <sub>2</sub> : d809, e120           |
| C <sub>12</sub>                                                             | C <sub>12</sub> H <sub>12</sub> O <sub>2</sub> Si: d769                       | C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> : c314                 |
|                                                                             | C <sub>12</sub> H <sub>12</sub> O <sub>3</sub> : e78                          | C <sub>12</sub> H <sub>25</sub> Br: b327                              |
| C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub> S <sub>2</sub> : b226        | C <sub>12</sub> H <sub>12</sub> O <sub>6</sub> : t193, t360                   | C <sub>12</sub> H <sub>25</sub> Cl: e119                              |
| C <sub>12</sub> H <sub>6</sub> Br <sub>4</sub> O <sub>4</sub> S: s28        | C <sub>12</sub> H <sub>13</sub> N: t68                                        | C <sub>12</sub> H <sub>25</sub> Cl <sub>3</sub> Si: d821              |
| C <sub>12</sub> H <sub>6</sub> O <sub>3</sub> : n8                          | C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> : d34                          | C <sub>12</sub> H <sub>25</sub> I: i30                                |
| C <sub>12</sub> H <sub>6</sub> O <sub>12</sub> : b20                        | C <sub>12</sub> H <sub>13</sub> NO <sub>3</sub> S: p272                       | C <sub>12</sub> H <sub>25</sub> N: c340                               |
| C <sub>12</sub> H <sub>7</sub> Cl <sub>6</sub> O: d296                      | C <sub>12</sub> H <sub>14</sub> : d467                                        | C <sub>12</sub> H <sub>25</sub> N <sub>3</sub> : i6                   |
| C <sub>12</sub> H <sub>8</sub> : a3                                         | C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> : d46                          | C <sub>12</sub> H <sub>26</sub> : d803                                |
| C <sub>12</sub> H <sub>8</sub> Br <sub>2</sub> : d80                        | C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S: s22          | C <sub>12</sub> H <sub>26</sub> O: d414, d810                         |
| C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> OS: b172                     | C <sub>12</sub> H <sub>14</sub> O: b525                                       | C <sub>12</sub> H <sub>26</sub> O <sub>2</sub> : d806, d807           |
| C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub> S: b171, c223 | C <sub>12</sub> H <sub>14</sub> O <sub>3</sub> : e179                         | C <sub>12</sub> H <sub>26</sub> O <sub>3</sub> : b151                 |
| C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> : p63                         | C <sub>12</sub> H <sub>14</sub> O <sub>4</sub> : d391                         | C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> : d460, t91            |
| C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> S: b216        | C <sub>12</sub> H <sub>15</sub> NO: b121                                      | C <sub>12</sub> H <sub>26</sub> O <sub>3</sub> S: d820                |
| C <sub>12</sub> H <sub>8</sub> O: d66                                       | C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> : t196          | C <sub>12</sub> H <sub>26</sub> O <sub>5</sub> : t53                  |
| C <sub>12</sub> H <sub>8</sub> S: d67                                       | C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> S: d42          | C <sub>12</sub> H <sub>26</sub> S: d808                               |
| C <sub>12</sub> H <sub>9</sub> Br: b273                                     | C <sub>12</sub> H <sub>16</sub> : b598, c376, m221                            | C <sub>12</sub> H <sub>27</sub> Al: t322                              |
| C <sub>12</sub> H <sub>9</sub> BrO: b325, b398                              | C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> : p64                          | C <sub>12</sub> H <sub>27</sub> B: t209                               |
| C <sub>12</sub> H <sub>9</sub> ClO <sub>2</sub> S: c221                     | C <sub>12</sub> H <sub>16</sub> O <sub>3</sub> : d298                         | C <sub>12</sub> H <sub>27</sub> BO <sub>3</sub> : t207                |
| C <sub>12</sub> H <sub>9</sub> N: c6, d751, n16                             | C <sub>12</sub> H <sub>17</sub> N: b120                                       | C <sub>12</sub> H <sub>27</sub> ClSn: t213                            |
| C <sub>12</sub> H <sub>9</sub> NO: b73, b74, b75                            | C <sub>12</sub> H <sub>17</sub> NO: d402                                      | C <sub>12</sub> H <sub>27</sub> N: d413, d818, t208                   |
| C <sub>12</sub> H <sub>9</sub> NO <sub>2</sub> : n46, n47                   | C <sub>12</sub> H <sub>18</sub> : c338, d473, d474, p116, t453                | C <sub>12</sub> H <sub>27</sub> O <sub>3</sub> P: t212                |
| C <sub>12</sub> H <sub>9</sub> NO <sub>3</sub> : n68, n69                   | C <sub>12</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>4</sub> OS: t135       | C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P: t211                |
| C <sub>12</sub> H <sub>9</sub> NS: p67                                      | C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> : p186                         | C <sub>12</sub> H <sub>28</sub> BrN: t130                             |
| C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub> : d717         | C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> : i94           | C <sub>12</sub> H <sub>28</sub> N <sub>2</sub> : d804                 |
| C <sub>12</sub> H <sub>10</sub> : a2, b138                                  | C <sub>12</sub> H <sub>18</sub> O: b552, d479, e4                             | C <sub>12</sub> H <sub>28</sub> O <sub>4</sub> Ti: t164, t165         |
| C <sub>12</sub> H <sub>10</sub> ClN: a145                                   | C <sub>12</sub> H <sub>18</sub> O <sub>2</sub> : b550                         | C <sub>12</sub> H <sub>28</sub> Sn: t215                              |
| C <sub>12</sub> H <sub>10</sub> ClO <sub>3</sub> P: c748                    | C <sub>12</sub> H <sub>18</sub> O <sub>3</sub> : o41                          | C <sub>12</sub> H <sub>29</sub> N: t323                               |
| C <sub>12</sub> H <sub>10</sub> ClP: c118                                   | C <sub>12</sub> H <sub>18</sub> O <sub>4</sub> : b463, h58                    | C <sub>12</sub> H <sub>29</sub> N <sub>3</sub> : b196                 |
| C <sub>12</sub> H <sub>10</sub> Cl <sub>2</sub> Si: d223                    | C <sub>12</sub> H <sub>19</sub> N: d471                                       |                                                                       |
| C <sub>12</sub> H <sub>10</sub> Hg: d758                                    | C <sub>12</sub> H <sub>20</sub> O <sub>2</sub> : b202, b296, e112, g3, L12    | C <sub>13</sub>                                                       |
| C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> : a312                       | C <sub>12</sub> H <sub>20</sub> O <sub>3</sub> Si: p160                       |                                                                       |
| C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O: n79, p90                  | C <sub>12</sub> H <sub>20</sub> O <sub>4</sub> : d154                         | C <sub>13</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub> : h29   |
| C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> : n51         | C <sub>12</sub> H <sub>20</sub> O <sub>4</sub> Sn: d179                       | C <sub>13</sub> H <sub>8</sub> ClNO <sub>3</sub> : c198               |
| C <sub>12</sub> H <sub>10</sub> N <sub>3</sub> O <sub>3</sub> P: d764       | C <sub>12</sub> H <sub>20</sub> O <sub>5</sub> : t278                         | C <sub>13</sub> H <sub>8</sub> Cl <sub>2</sub> O: d205                |
| C <sub>12</sub> H <sub>10</sub> O: d753, m322, m323, p135, p136             | C <sub>12</sub> H <sub>21</sub> N: t446                                       | C <sub>13</sub> H <sub>8</sub> O: f3                                  |
| C <sub>12</sub> H <sub>10</sub> OS: d772                                    | C <sub>12</sub> H <sub>21</sub> NO <sub>3</sub> Si: t345                      | C <sub>13</sub> H <sub>8</sub> OS: t162                               |
| C <sub>12</sub> H <sub>10</sub> O <sub>2</sub> : d436, h89, n14, n15        | C <sub>12</sub> H <sub>21</sub> N <sub>3</sub> : t429                         | C <sub>13</sub> H <sub>8</sub> O <sub>2</sub> : x3                    |
| C <sub>12</sub> H <sub>10</sub> O <sub>2</sub> S: d771, t145                | C <sub>12</sub> H <sub>22</sub> : c339, d288                                  | C <sub>13</sub> H <sub>9</sub> BrO: b267                              |
| C <sub>12</sub> H <sub>10</sub> O <sub>3</sub> : n12                        | C <sub>12</sub> H <sub>22</sub> BCl: c95                                      | C <sub>13</sub> H <sub>9</sub> ClO: c56, c57                          |
| C <sub>12</sub> H <sub>10</sub> O <sub>3</sub> S: b142                      | C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub> : d45           | C <sub>13</sub> H <sub>9</sub> ClO <sub>2</sub> : c151                |
| C <sub>12</sub> H <sub>10</sub> O <sub>4</sub> : q1                         | C <sub>12</sub> H <sub>22</sub> O: c337, e5                                   | C <sub>3</sub> H <sub>9</sub> N: a60                                  |
| C <sub>12</sub> H <sub>10</sub> O <sub>4</sub> S: s30                       | C <sub>12</sub> H <sub>22</sub> O <sub>2</sub> : d811, e172, m14              | C <sub>13</sub> H <sub>10</sub> : f2                                  |
| C <sub>12</sub> H <sub>10</sub> S: d770                                     | C <sub>12</sub> H <sub>22</sub> O <sub>3</sub> : h65                          | C <sub>13</sub> H <sub>10</sub> ClNO: a140, a141, d745                |
| C <sub>12</sub> H <sub>10</sub> S <sub>2</sub> : d750                       | C <sub>12</sub> H <sub>22</sub> O <sub>4</sub> : d168, d384, d597, d787, d805 | C <sub>13</sub> H <sub>10</sub> Cl <sub>2</sub> : d221                |
| C <sub>12</sub> H <sub>10</sub> Se <sub>2</sub> : d749                      | C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> : d174                         | C <sub>13</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub> : m243 |
| C <sub>12</sub> H <sub>11</sub> N: a130, a131, b122, b123, d743             |                                                                               | C <sub>13</sub> H <sub>10</sub> F <sub>2</sub> : b195                 |
| C <sub>12</sub> H <sub>11</sub> NO: h115, n13, p70                          |                                                                               | C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> : p91                  |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $C_{13}H_{10}N_2O_3$ : a235<br>$C_{13}H_{10}O$ : b53, x1<br>$C_{13}H_{10}O_2$ : b139, h103, m68, p92<br>$C_{13}H_{10}O_3$ : d435, d747, p154, r5<br>$C_{13}H_{10}O_4$ : t320<br>$C_{13}H_{10}O_5$ : t88<br>$C_{13}H_{11}Br$ : b326<br>$C_{13}H_{11}Cl$ : c116<br>$C_{13}H_{11}N$ : b102<br>$C_{13}H_{11}NO$ : a124, b5<br>$C_{13}H_{11}NO_3$ : p87<br>$C_{13}H_{12}$ : d759<br>$C_{13}H_{12}NO_2$ : b112<br>$C_{13}H_{12}N_2$ : b54, d754<br>$C_{13}H_{12}N_2O$ : d775<br>$C_{13}H_{12}N_2S$ : d774, t141<br>$C_{13}H_{12}N_4O$ : d746, p89<br>$C_{13}H_{12}N_4S$ : d773<br>$C_{13}H_{12}O$ : d760, h116, h117, m63, p76<br>$C_{13}H_{12}O_2$ : m320<br>$C_{13}H_{12}O_4$ : d32<br>$C_{13}H_{12}S$ : b118<br>$C_{13}H_{13}ClSi$ : c117<br>$C_{13}H_{13}N$ : d761, m238, p93<br>$C_{13}H_{13}NO_2$ : t187<br>$C_{13}H_{13}N_3$ : d755<br>$C_{13}H_{14}N_2$ : d35, m249<br>$C_{13}H_{14}N_2O_3$ : a59<br>$C_{13}H_{14}N_4O$ : d746<br>$C_{13}H_{15}NO$ : i96<br>$C_{13}H_{16}O_3$ : e79<br>$C_{13}H_{16}O_4$ : d389<br>$C_{13}H_{17}NO_2$ : e82<br>$C_{13}H_{18}O_3$ : b117<br>$C_{13}H_{18}O_5$ : t267<br>$C_{13}H_{20}$ : p115<br>$C_{13}H_{20}O$ : i58, i59<br>$C_{13}H_{22}ClN$ : b130<br>$C_{13}H_{22}N_2$ : d290<br>$C_{13}H_{22}O_3Si$ : b129<br>$C_{13}H_{24}O_2$ : e273, i86<br>$C_{13}H_{24}O_4$ : d337<br>$C_{13}H_{26}$ : t265<br>$C_{13}H_{26}N_2$ : m246, t369<br>$C_{13}H_{26}O$ : t263, t264<br>$C_{13}H_{26}O_2$ : e232, t262<br>$C_{13}H_{27}Br$ : b433<br>$C_{13}H_{28}$ : t261<br>$C_{13}H_{28}O_4$ : t431<br>$C_{13}H_{29}Cl$ : c250<br>$C_{13}H_{29}NO_4$ : b176<br>$C_{13}H_{30}OSn$ : t216 | $C_{14}$<br>$C_{14}H_6Cl_2O_2$ : d193<br>$C_{14}H_7ClO_2$ : c41, c42<br>$C_{14}H_8O_2$ : a298<br>$C_{14}H_8O_4$ : d426<br>$C_{14}H_9Br$ : b391<br>$C_{14}H_9ClO_3$ : c63<br>$C_{14}H_9Cl_5$ : b173<br>$C_{14}H_9NO_2$ : a108, a109<br>$C_{14}H_{10}$ : a297, d742, p62<br>$C_{14}H_{10}ClNO_3$ : a144<br>$C_{14}H_{10}Cl_2O_4$ : b168<br>$C_{14}H_{10}Cl_4$ : b169<br>$C_{14}H_{10}N_2O_2$ : d36, d37, d38, d39<br>$C_{14}H_{10}O_2$ : b35<br>$C_{14}H_{10}O_3$ : b45, b64, x2<br>$C_{14}H_{10}O_4$ : b141, d69, b71a<br>$C_{14}H_{10}O_4S_2$ : d796<br>$C_{14}H_{11}N$ : d741, p123<br>$C_{14}H_{11}NOS$ : a50<br>$C_{14}H_{12}$ : d415, s9<br>$C_{14}H_{12}Cl_2O$ : b170<br>$C_{14}H_{12}N_2O$ : b38<br>$C_{14}H_{12}N_2O_2$ : b36<br>$C_{14}H_{12}O$ : a34, d26, m145<br>$C_{14}H_{12}O_2$ : b46, b83, b84, b113, d740<br>$C_{14}H_{12}O_3$ : b37, b100, b125, h144<br>$C_{14}H_{13}ClO$ : c169<br>$C_{14}H_{13}N$ : e104, i9<br>$C_{14}H_{13}NO$ : b82, d739<br>$C_{14}H_{13}NO_2$ : b50<br>$C_{14}H_{14}$ : d752<br>$C_{14}H_{14}N_2$ : a168<br>$C_{14}H_{14}N_2O$ : m240<br>$C_{14}H_{14}N_2O_3$ : a315<br>$C_{14}H_{14}O$ : d73<br>$C_{14}H_{14}OS$ : b223<br>$C_{14}H_{14}O_2$ : b114<br>$C_{14}H_{14}O_4$ : d33<br>$C_{14}H_{14}S_2$ : b222, d72<br>$C_{14}H_{15}N$ : d71<br>$C_{14}H_{16}N_2O_4$ : b207<br>$C_{14}H_{16}O_2Si$ : d503<br>$C_{14}H_{16}O_4$ : d340<br>$C_{14}H_{18}N_2O_2$ : m132<br>$C_{14}H_{18}O$ : p56<br>$C_{14}H_{18}O_4$ : d343<br>$C_{14}H_{18}O_7$ : p21<br>$C_{14}H_{19}O_3$ : d293<br>$C_{14}H_{22}O$ : d160, d161, d162, d163 | $C_{14}H_{22}O_2$ : d145<br>$C_{14}H_{22}O_3$ : d153<br>$C_{14}H_{22}O_4$ : h59<br>$C_{14}H_{22}O_6$ : t281<br>$C_{14}H_{22}O_7$ : t52<br>$C_{14}H_{23}N$ : d142<br>$C_{14}H_{23}N_3O_{10}$ : d299<br>$C_{14}H_{26}O_2$ : i87<br>$C_{14}H_{26}O_3$ : h10<br>$C_{14}H_{26}O_4$ : d152, d395, d459<br>$C_{14}H_{27}ClO$ : t46<br>$C_{14}H_{28}$ : t47<br>$C_{14}H_{28}O$ : d822<br>$C_{14}H_{28}O_2$ : d815, e272, t44<br>$C_{14}H_{29}Br$ : b423<br>$C_{14}H_{29}O_4$ : b156<br>$C_{14}H_{30}$ : t43<br>$C_{14}H_{30}O$ : t45<br>$C_{14}H_{30}O_2Sn$ : d136<br>$C_{14}H_{31}N$ : d602<br>$C_{14}H_{32}N_2O_4$ : t90<br>$C_{14}H_{32}OSn$ : t214                                                                                                                                                                                                                                                              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | $C_{15}$<br>$C_{15}H_{10}N_2O_2$ : m247<br>$C_{15}H_{10}O_2$ : b105, m136, p122<br>$C_{15}H_{11}NO$ : d762<br>$C_{15}H_{11}NO_2$ : m128<br>$C_{15}H_{12}N_2O_2$ : d756<br>$C_{15}H_{12}O$ : c23<br>$C_{15}H_{12}O_2$ : d68<br>$C_{15}H_{13}NO$ : a13<br>$C_{15}H_{14}O$ : d767<br>$C_{15}H_{14}O_2$ : b49, d768, h169<br>$C_{15}H_{14}O_3$ : b116, m239<br>$C_{15}H_{16}O$ : c316a<br>$C_{15}H_{16}O_2$ : e189, i113<br>$C_{15}H_{17}N$ : b96a<br>$C_{15}H_{17}N_3$ : d797<br>$C_{15}H_{20}O_6$ : e184<br>$C_{15}H_{22}O_3$ : d117, e174<br>$C_{15}H_{22}O_5$ : o46<br>$C_{15}H_{23}N$ : b583<br>$C_{15}H_{24}$ : t327<br>$C_{15}H_{24}O$ : d156<br>$C_{15}H_{26}O_6$ : g20<br>$C_{15}H_{28}O_2$ : d816, i112<br>$C_{15}H_{29}N$ : p12<br>$C_{15}H_{30}N_2$ : t368<br>$C_{15}H_{30}O$ : p13<br>$C_{15}H_{30}O_2$ : m428<br>$C_{15}H_{32}$ : p11<br>$C_{15}H_{32}O_{10}$ : t409<br>$C_{15}H_{33}NO_6$ : t443 |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)*The alphanumeric designations are keyed to Table 1.15.*

| C <sub>16</sub>                                                                     |                                                                       |                                                                       |
|-------------------------------------------------------------------------------------|-----------------------------------------------------------------------|-----------------------------------------------------------------------|
| C <sub>16</sub> H <sub>10</sub> : b52, f1, p255                                     | C <sub>17</sub> H <sub>16</sub> O <sub>4</sub> : d75, p194            | C <sub>18</sub> H <sub>36</sub> : o8                                  |
| C <sub>16</sub> H <sub>11</sub> NO <sub>2</sub> : p153                              | C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> : p193  | C <sub>18</sub> H <sub>36</sub> O: e13, o12                           |
| C <sub>16</sub> H <sub>12</sub> N <sub>4</sub> O <sub>9</sub> S <sub>2</sub> : t5   | C <sub>17</sub> H <sub>18</sub> O <sub>2</sub> : b589                 | C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> : e157, o5             |
| C <sub>16</sub> H <sub>13</sub> N: p132, p133                                       | C <sub>17</sub> H <sub>18</sub> O <sub>3</sub> : b592                 | C <sub>18</sub> H <sub>37</sub> Br: b384                              |
| C <sub>16</sub> H <sub>14</sub> : d744, e71                                         | C <sub>17</sub> H <sub>18</sub> O <sub>4</sub> : b203                 | C <sub>18</sub> H <sub>37</sub> Cl: c203a                             |
| C <sub>16</sub> H <sub>14</sub> O <sub>2</sub> : b93                                | C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O: b178                | C <sub>18</sub> H <sub>37</sub> Cl <sub>3</sub> Si: o17               |
| C <sub>16</sub> H <sub>14</sub> O <sub>6</sub> S: s29                               | C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O <sub>6</sub> : r8    | C <sub>18</sub> H <sub>37</sub> I: i43                                |
| C <sub>16</sub> H <sub>16</sub> O <sub>2</sub> : b47                                | C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub> : b291                | C <sub>18</sub> H <sub>37</sub> N: o9                                 |
| C <sub>16</sub> H <sub>16</sub> O <sub>3</sub> : d515                               | C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> : m245                 | C <sub>18</sub> H <sub>37</sub> NO: o2                                |
| C <sub>16</sub> H <sub>18</sub> ClN <sub>3</sub> S: m248                            | C <sub>17</sub> H <sub>23</sub> NO <sub>3</sub> : a305                | C <sub>18</sub> H <sub>38</sub> : o3                                  |
| C <sub>16</sub> H <sub>19</sub> ClSi: b537                                          | C <sub>17</sub> H <sub>24</sub> O <sub>6</sub> : b492                 | C <sub>18</sub> H <sub>38</sub> O: o6                                 |
| C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> : d74                                | C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub> : m15                 | C <sub>18</sub> H <sub>38</sub> S: o4                                 |
| C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O: b178                              | C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub> : e170                | C <sub>18</sub> H <sub>39</sub> ClSi: t315                            |
| C <sub>16</sub> H <sub>20</sub> O <sub>2</sub> Si: d302                             | C <sub>17</sub> H <sub>28</sub> NO: d149                              | C <sub>18</sub> H <sub>39</sub> N: o15, t313                          |
| C <sub>16</sub> H <sub>22</sub> O <sub>4</sub> : d165, d410                         | C <sub>17</sub> H <sub>28</sub> O <sub>7</sub> : d181                 | C <sub>18</sub> H <sub>39</sub> O <sub>7</sub> P: t435                |
| C <sub>16</sub> H <sub>22</sub> O <sub>11</sub> : g9                                | C <sub>17</sub> H <sub>34</sub> O <sub>2</sub> : m269a, i131          | C <sub>18</sub> H <sub>40</sub> Si: t316                              |
| C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> : d150                               | C <sub>17</sub> H <sub>34</sub> O <sub>4</sub> : b160                 |                                                                       |
| C <sub>16</sub> H <sub>26</sub> O <sub>3</sub> : d814                               | C <sub>17</sub> H <sub>36</sub> : h1                                  | C <sub>19</sub>                                                       |
| C <sub>16</sub> H <sub>26</sub> O <sub>7</sub> : t54                                | C <sub>17</sub> H <sub>36</sub> O: h1a                                | C <sub>19</sub> H <sub>15</sub> Br: b440, t417                        |
| C <sub>16</sub> H <sub>28</sub> O: c346                                             | C <sub>17</sub> H <sub>37</sub> N: m236                               | C <sub>19</sub> H <sub>15</sub> Cl: c267, t418                        |
| C <sub>16</sub> H <sub>30</sub> O <sub>2</sub> : d819                               |                                                                       | C <sub>19</sub> H <sub>16</sub> : t415                                |
| C <sub>16</sub> H <sub>30</sub> O <sub>4</sub> : b158, d157, d167, d360             | C <sub>18</sub>                                                       | C <sub>19</sub> H <sub>16</sub> O: t416                               |
| C <sub>16</sub> H <sub>32</sub> : h37                                               | C <sub>18</sub> H <sub>12</sub> : b6, b7                              | C <sub>19</sub> H <sub>18</sub> BrP: m458                             |
| C <sub>16</sub> H <sub>32</sub> O: e10                                              | C <sub>18</sub> H <sub>12</sub> N <sub>5</sub> O <sub>6</sub> : d766  | C <sub>19</sub> H <sub>19</sub> N <sub>7</sub> O <sub>6</sub> : f31   |
| C <sub>16</sub> H <sub>32</sub> O <sub>2</sub> : h34                                | C <sub>18</sub> H <sub>14</sub> : t7, t8, t9                          | C <sub>19</sub> H <sub>20</sub> Br <sub>4</sub> O <sub>4</sub> : i110 |
| C <sub>16</sub> H <sub>33</sub> Br: b345                                            | C <sub>18</sub> H <sub>14</sub> O <sub>8</sub> : d70                  | C <sub>19</sub> H <sub>20</sub> O <sub>4</sub> : b88                  |
| C <sub>16</sub> H <sub>33</sub> Cl: c148                                            | C <sub>18</sub> H <sub>15</sub> As: t412                              | C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O: c276                |
| C <sub>16</sub> H <sub>33</sub> I: i35                                              | C <sub>18</sub> H <sub>15</sub> B: t414                               | C <sub>19</sub> H <sub>30</sub> O <sub>5</sub> : m252                 |
| C <sub>16</sub> H <sub>33</sub> NO: d359                                            | C <sub>18</sub> H <sub>15</sub> ClSn: c268, t425                      | C <sub>19</sub> H <sub>31</sub> N: d24                                |
| C <sub>16</sub> H <sub>34</sub> : h4, h31, h36                                      | C <sub>18</sub> H <sub>15</sub> N: t410                               | C <sub>19</sub> H <sub>34</sub> ClN: b127                             |
| C <sub>16</sub> H <sub>34</sub> O: d729, h35                                        | C <sub>18</sub> H <sub>15</sub> NO <sub>2</sub> : e116                | C <sub>19</sub> H <sub>36</sub> O <sub>2</sub> : m347                 |
| C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> : h32                                | C <sub>18</sub> H <sub>15</sub> N <sub>3</sub> Si: a310               | C <sub>19</sub> H <sub>37</sub> NO: o16                               |
| C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> : b157                               | C <sub>18</sub> H <sub>15</sub> OP: t421                              | C <sub>19</sub> H <sub>38</sub> O <sub>2</sub> : i109, m346           |
| C <sub>16</sub> H <sub>34</sub> S: d720, h33                                        | C <sub>18</sub> H <sub>15</sub> O <sub>3</sub> P: t422                | C <sub>19</sub> H <sub>40</sub> : n89, t114                           |
| C <sub>16</sub> H <sub>35</sub> N: d728, h37                                        | C <sub>18</sub> H <sub>15</sub> O <sub>4</sub> P: t419                |                                                                       |
| C <sub>16</sub> H <sub>35</sub> O <sub>3</sub> P: b192                              | C <sub>18</sub> H <sub>15</sub> P: t420                               | C <sub>20</sub>                                                       |
| C <sub>16</sub> H <sub>36</sub> BF <sub>4</sub> N: t25                              | C <sub>18</sub> H <sub>15</sub> Sb: t411                              | C <sub>20</sub> H <sub>10</sub> Br <sub>2</sub> O <sub>5</sub> : d105 |
| C <sub>16</sub> H <sub>36</sub> BrN: t21                                            | C <sub>18</sub> H <sub>16</sub> OSn: t426                             | C <sub>20</sub> H <sub>12</sub> : b56, b57, d65                       |
| C <sub>16</sub> H <sub>36</sub> BrP: t29                                            | C <sub>18</sub> H <sub>16</sub> O <sub>2</sub> : b520, d280           | C <sub>20</sub> H <sub>12</sub> O <sub>5</sub> : f4                   |
| C <sub>16</sub> H <sub>36</sub> Br <sub>3</sub> N: t26                              | C <sub>18</sub> H <sub>16</sub> Si: t423                              | C <sub>20</sub> H <sub>14</sub> O <sub>4</sub> : d765, p66            |
| C <sub>16</sub> H <sub>36</sub> ClN: t22                                            | C <sub>18</sub> H <sub>18</sub> O <sub>3</sub> : e81                  | C <sub>20</sub> H <sub>15</sub> Br: b439                              |
| C <sub>16</sub> H <sub>36</sub> IN: t24                                             | C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> : e152  | C <sub>20</sub> H <sub>18</sub> O <sub>2</sub> Sn: t424               |
| C <sub>16</sub> H <sub>36</sub> O <sub>4</sub> Si: t28                              | C <sub>18</sub> H <sub>20</sub> O: b548                               | C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> : b2                   |
| C <sub>16</sub> H <sub>36</sub> Sn: t30                                             | C <sub>18</sub> H <sub>20</sub> O <sub>2</sub> : b48                  | C <sub>20</sub> H <sub>20</sub> BrOP: h136                            |
| C <sub>16</sub> H <sub>37</sub> NO <sub>4</sub> S: t23                              | C <sub>18</sub> H <sub>22</sub> : b182                                | C <sub>20</sub> H <sub>32</sub> O <sub>5</sub> : d782                 |
|                                                                                     | C <sub>18</sub> H <sub>26</sub> O <sub>6</sub> : e185                 | C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> : q2    |
|                                                                                     | C <sub>18</sub> H <sub>30</sub> O: t210                               | C <sub>20</sub> H <sub>26</sub> O <sub>4</sub> : d291                 |
|                                                                                     | C <sub>18</sub> H <sub>30</sub> O <sub>2</sub> : o7                   | C <sub>20</sub> H <sub>27</sub> O <sub>3</sub> P: i90                 |
|                                                                                     | C <sub>18</sub> H <sub>32</sub> N <sub>4</sub> O <sub>14</sub> : d364 | C <sub>20</sub> H <sub>30</sub> O <sub>2</sub> : a1                   |
|                                                                                     | C <sub>18</sub> H <sub>32</sub> O <sub>2</sub> : o1                   | C <sub>20</sub> H <sub>30</sub> O <sub>6</sub> : b184                 |
|                                                                                     | C <sub>18</sub> H <sub>32</sub> O <sub>16</sub> : r1                  | C <sub>20</sub> H <sub>31</sub> N: d20                                |
|                                                                                     | C <sub>18</sub> H <sub>33</sub> ClO: o13                              | C <sub>20</sub> H <sub>34</sub> O <sub>4</sub> : b159                 |
|                                                                                     | C <sub>18</sub> H <sub>34</sub> O <sub>2</sub> : o10, o11             | C <sub>20</sub> H <sub>36</sub> O <sub>2</sub> : e229                 |
|                                                                                     | C <sub>18</sub> H <sub>34</sub> O <sub>4</sub> : d143                 |                                                                       |
| C <sub>17</sub>                                                                     |                                                                       |                                                                       |
| C <sub>17</sub> H <sub>12</sub> O <sub>3</sub> : p118, p119                         |                                                                       |                                                                       |
| C <sub>17</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub> : p173 |                                                                       |                                                                       |
| C <sub>17</sub> H <sub>15</sub> N <sub>2</sub> O: d355                              |                                                                       |                                                                       |

**TABLE 1.14** Empirical Formula Index of Organic Compounds (*Continued*)

The alphanumeric designations are keyed to Table 1.15.

|                                                                                       |                                                                          |                                                                      |
|---------------------------------------------------------------------------------------|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| C <sub>20</sub> H <sub>38</sub> O <sub>2</sub> : e230                                 | C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> : b447     | C <sub>27</sub> H <sub>42</sub> O: c274                              |
| C <sub>20</sub> H <sub>38</sub> O <sub>4</sub> : b187                                 | C <sub>23</sub> H <sub>42</sub> O <sub>2</sub> : b581a                   | C <sub>27</sub> H <sub>50</sub> ClN: b96                             |
| C <sub>20</sub> H <sub>40</sub> : i2                                                  |                                                                          | C <sub>28</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>3</sub> : r6 |
| C <sub>20</sub> H <sub>40</sub> O: o18                                                | C <sub>24</sub> to C <sub>29</sub>                                       | C <sub>28</sub> H <sub>32</sub> : t127                               |
| C <sub>20</sub> H <sub>42</sub> : i1                                                  |                                                                          | C <sub>28</sub> H <sub>50</sub> O <sub>8</sub> : t314                |
| C <sub>21</sub> to C <sub>23</sub>                                                    | C <sub>24</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> : b218     | C <sub>28</sub> H <sub>54</sub> O <sub>6</sub> Sn: b601              |
|                                                                                       | C <sub>24</sub> H <sub>18</sub> : t413                                   | C <sub>29</sub> H <sub>44</sub> O <sub>2</sub> : m244                |
|                                                                                       | C <sub>24</sub> H <sub>20</sub> BNA: t126                                | C <sub>29</sub> H <sub>50</sub> O <sub>7</sub> : p20                 |
|                                                                                       | C <sub>24</sub> H <sub>20</sub> Sn: t128                                 | C <sub>30</sub> to C <sub>57</sub>                                   |
|                                                                                       | C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub> : e169                   |                                                                      |
|                                                                                       | C <sub>24</sub> H <sub>38</sub> O <sub>4</sub> : b193, d374, d466, d466a | C <sub>30</sub> H <sub>43</sub> FO <sub>2</sub> P: e188              |
| C <sub>21</sub> H <sub>15</sub> NO: b143                                              | C <sub>24</sub> H <sub>40</sub> O <sub>5</sub> : c275                    | C <sub>30</sub> H <sub>46</sub> O <sub>2</sub> : e187                |
| C <sub>21</sub> H <sub>21</sub> N: t198                                               | C <sub>24</sub> H <sub>46</sub> O <sub>4</sub> : d725, d812              | C <sub>30</sub> H <sub>50</sub> : s8                                 |
| C <sub>21</sub> H <sub>21</sub> O <sub>4</sub> P: t452                                | C <sub>24</sub> H <sub>50</sub> : t41                                    | C <sub>30</sub> H <sub>58</sub> O <sub>4</sub> S: d295               |
| C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> : s10                   | C <sub>24</sub> H <sub>51</sub> N: t406                                  | C <sub>30</sub> H <sub>62</sub> : s7                                 |
| C <sub>21</sub> H <sub>24</sub> O <sub>2</sub> : b144                                 | C <sub>24</sub> H <sub>51</sub> O <sub>3</sub> P: t438                   | C <sub>30</sub> H <sub>63</sub> O <sub>3</sub> P: t324               |
| C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O: b177                                | C <sub>24</sub> H <sub>54</sub> OSn <sub>2</sub> : b224                  | C <sub>32</sub> H <sub>64</sub> O <sub>4</sub> Sn: d178              |
| C <sub>21</sub> H <sub>36</sub> O: p14                                                | C <sub>25</sub> H <sub>30</sub> ClN <sub>3</sub> : c315                  | C <sub>32</sub> H <sub>66</sub> : d823                               |
| C <sub>21</sub> H <sub>40</sub> O <sub>2</sub> : o14                                  | C <sub>25</sub> H <sub>34</sub> Cl <sub>6</sub> O <sub>4</sub> : b189    | C <sub>36</sub> H <sub>75</sub> O <sub>3</sub> P: d726               |
| C <sub>21</sub> H <sub>45</sub> N <sub>3</sub> O <sub>12</sub> Si <sub>3</sub> : t448 | C <sub>25</sub> H <sub>48</sub> O <sub>4</sub> : d465                    | C <sub>39</sub> H <sub>74</sub> O <sub>6</sub> : g21                 |
| C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub> : a306                  | C <sub>26</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S: b153    | C <sub>40</sub> H <sub>82</sub> O <sub>6</sub> P <sub>2</sub> : b217 |
| C <sub>22</sub> H <sub>26</sub> O: b181                                               | C <sub>26</sub> H <sub>42</sub> O <sub>2</sub> : d138                    | C <sub>42</sub> H <sub>82</sub> O <sub>4</sub> S: d727               |
| C <sub>22</sub> H <sub>30</sub> O <sub>2</sub> S: t140                                | C <sub>26</sub> H <sub>42</sub> O <sub>4</sub> : d464                    | C <sub>45</sub> H <sub>86</sub> O <sub>6</sub> : g25                 |
| C <sub>22</sub> H <sub>34</sub> O <sub>4</sub> : b547, d463                           | C <sub>26</sub> H <sub>47</sub> O <sub>3</sub> P: d462                   | C <sub>51</sub> H <sub>98</sub> O <sub>6</sub> : g24                 |
| C <sub>22</sub> H <sub>42</sub> O <sub>8</sub> : b152                                 | C <sub>26</sub> H <sub>46</sub> O <sub>8</sub> : t312                    | C <sub>55</sub> H <sub>98</sub> O <sub>6</sub> P <sub>2</sub> : i111 |
| C <sub>22</sub> H <sub>44</sub> O <sub>2</sub> : b581, i75                            | C <sub>26</sub> H <sub>50</sub> O <sub>4</sub> : b190                    | C <sub>57</sub> H <sub>104</sub> O <sub>6</sub> : g23                |
| C <sub>22</sub> H <sub>46</sub> : d801                                                |                                                                          |                                                                      |
| C <sub>22</sub> H <sub>46</sub> O: d802                                               |                                                                          |                                                                      |
| C <sub>22</sub> H <sub>48</sub> N <sub>2</sub> : t27                                  |                                                                          |                                                                      |
| C <sub>23</sub> H <sub>18</sub> BrO <sub>2</sub> P: c18                               |                                                                          |                                                                      |

**TABLE 1.15** Physical Constants of Organic Compounds

See also the special tables of polymers, rubbers, fats, oils, and waxes.

*Names* of the compounds in the table starting on p. 1.76 are arranged alphabetically. Usually substitutive nomenclature is employed; exceptions generally involve ethers, sulfides, sulfones, and sulfoxides. Each compound is given a number within its letter classification; thus compound c209 is 3-chlorophenol. Section 1.1, Nomenclature of Organic Compounds, should be consulted to familiarize oneself with present nomenclature systems.

*Synonyms or Alternate Names* are found at the bottom of each spread in their alphabetical listing; the number following the same refers to the numerical place of this compound in the table. For example, epichlorohydrin, c120, indicates that this compound is found listed under the name 1-chloro-2,3-epoxypropane.

*Formulas* are presented in semistructural form when no ambiguity is possible. Complicated systems are drawn in complete structural form and located at the bottom of each page and keyed to the number of the entry.

*Beilstein Reference.* In this column is found the reference to the volume and page numbers of the fourth edition of Beilstein, *Handbuch der Organischen Chemie* (Springer-Verlag, New York, 1918). Thus the entry 9, 202 refers to an entry in volume 9 appearing on page 202. When the volume number has a superscript attached, reference is made to the appropriate supplementary volume. For example, 12<sup>2</sup>, 404 indicates that the compound will be found listed in the second supplement to volume 12 on page 404. The earliest Beilstein entry is listed. Supplementary information may be found in the supplements to the basic series; such coordinating references (series number, volume number, and page number of the main edition) along with the system number are found at the top of each *odd-numbered page*. Similarly, a back reference such as H93; E II 64; E III 190 in a volume of Supplementary Series IV means that previous items on this compound are found in the same volume of the



---

# SECTION 2

---

## GENERAL INFORMATION, CONVERSION TABLES, AND MATHEMATICS

---

|                                                                                                      |              |
|------------------------------------------------------------------------------------------------------|--------------|
| <b>2.1 GENERAL INFORMATION AND CONVERSION TABLES</b>                                                 | <b>2.3</b>   |
| Table 2.1 Fundamental Physical Constants                                                             | 2.3          |
| Table 2.2 Physical and Chemical Symbols and Definitions                                              | 2.6          |
| Table 2.3 Mathematical Symbols and Abbreviations                                                     | 2.23         |
| Table 2.4 SI Prefixes                                                                                | 2.24         |
| Table 2.5 Greek Alphabet                                                                             | 2.25         |
| Table 2.6 Abbreviations and Standard Letter Symbols                                                  | 2.26         |
| Table 2.7 Conversion Factors                                                                         | 2.35         |
| Table 2.8 Temperature Conversion Table                                                               | 2.54         |
| 2.1.1 Conversion of Thermometer Scales                                                               | 2.66         |
| 2.1.2 Density and Specific Gravity                                                                   | 2.66         |
| 2.1.3 Barometry and Barometric Corrections                                                           | 2.70         |
| Table 2.9 Barometer Temperature Correction—Metric Units                                              | 2.72         |
| Table 2.10 Barometric Latitude-Gravity Table—Metric Units                                            | 2.75         |
| Table 2.11 Barometric Correction for Gravity—Metric Units                                            | 2.77         |
| Table 2.12 Reduction of the Barometer to Sea Level—Metric Units                                      | 2.78         |
| Table 2.13 Viscosity Conversion Table                                                                | 2.82         |
| Table 2.14 Conversion of Weighings in Air to Weighings in Vacuo                                      | 2.83         |
| Table 2.15 Hydrometer Conversion Table                                                               | 2.85         |
| Table 2.16 Pressure Conversion Chart                                                                 | 2.87         |
| Table 2.17 Corrections to Be Added to Molar Values to Convert to Molal                               | 2.88         |
| Table 2.18 Molar Equivalent of One Liter of Gas at Various Temperatures and Pressures                | 2.88         |
| Table 2.19 Factors for Reducing Gas Volumes to Normal (Standard) Temperature and Pressure (760 mmHg) | 2.91         |
| Table 2.20 Values of Absorbance for Percent Absorption                                               | 2.96         |
| Table 2.21 Transmittance-Absorbance Conversion Table                                                 | 2.98         |
| Table 2.22 Wavenumber/Wavelength Conversion Table                                                    | 2.101        |
| <b>2.2 MATHEMATICAL TABLES</b>                                                                       | <b>2.102</b> |
| 2.2.1 Logarithms                                                                                     | 2.102        |
| Table 2.23 Derivatives and Differentiation                                                           | 2.104        |
| Table 2.24 Integrals                                                                                 | 2.105        |
| 2.2.2 Surface Areas and Volumes                                                                      | 2.109        |
| 2.2.3 Trigonometric Functions of an Angle $\alpha$                                                   | 2.113        |
| 2.2.4 Expansion in Series                                                                            | 2.115        |
| Table 2.25 Some Constants                                                                            | 2.117        |
| <b>2.3 STATISTICS IN CHEMICAL ANALYSIS</b>                                                           | <b>2.117</b> |
| 2.3.1 Introduction                                                                                   | 2.117        |
| 2.3.2 Errors in Quantitative Analysis                                                                | 2.118        |
| 2.3.3 Representation of Sets of Data                                                                 | 2.118        |
| 2.3.4 The Normal Distribution of Measurements                                                        | 2.119        |
| Figure 2.10 The Normal Distribution Curve                                                            | 2.119        |
| Table 2.26a Ordinates ( $Y$ ) of the Normal Distribution Curve at Values of $z$                      | 2.121        |
| Table 2.26b Areas Under the Normal Distribution Curve from 0 to $z$                                  | 2.122        |
| 2.3.5 Standard Deviation as a Measure of Dispersion                                                  | 2.121        |

|        |                                                                           |       |
|--------|---------------------------------------------------------------------------|-------|
| 2.3.6  | Student's Distribution or $t$ Test                                        | 2.123 |
|        | Table 2.27 Percentile Values for Student $t$ Distribution                 | 2.124 |
| 2.3.7  | Hypotheses About Means                                                    | 2.126 |
| 2.3.8  | The Chi-square ( $\chi^2$ ) Distribution                                  | 2.128 |
|        | Table 2.28 Percentile Values for the Chi-square ( $\chi^2$ ) Distribution | 2.129 |
| 2.3.9  | The $F$ Statistic                                                         | 2.130 |
|        | Table 2.29 $F$ Distribution                                               | 2.131 |
| 2.3.10 | Curve Fitting                                                             | 2.133 |
| 2.3.11 | Control Charts                                                            | 2.137 |
|        | Bibliography                                                              | 2.138 |

2.1 GENERAL INFORMATION AND CONVERSION TABLES

**TABLE 2.1** Fundamental Physical Constants  
*E. R. Cohen and B. N. Taylor, CODATA Bull. 63:1–49 (1986); J. Res. Nat. Bur. Standards, 92:85 (1987).*

| A. Defined values         |                 |                    |                                                                                                                                                                                                                                                                                    |
|---------------------------|-----------------|--------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Physical quantity         | Name of SI unit | Symbol for SI unit | Definition                                                                                                                                                                                                                                                                         |
| 1. Base SI units          |                 |                    |                                                                                                                                                                                                                                                                                    |
| Amount of substance       | mole            | mol                | Amount of substance which contains as many specified entities as there are atoms of carbon-12 in exactly 0.012 kg of that nuclide. The elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles. |
| Electric current          | ampere          | A                  | Magnitude of the current that, when flowing through each of two straight parallel conductors of infinite length, of negligible cross-section, separated by 1 meter in a vacuum, results in a force between the two wires of $2 \times 10^{-7}$ newton per meter of length.         |
| Length                    | meter           | m                  | Distance light travels in a vacuum during 1/299 792 458 of a second.                                                                                                                                                                                                               |
| Luminous intensity        | candela         | cd                 | Luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency $540 \times 10^{12}$ hertz and that has a radiant intensity in that direction of 1/683 watt per steradian.                                                                   |
| Mass                      | kilogram        | kg                 | Mass of a cylinder of platinum-iridium alloy kept at Paris.                                                                                                                                                                                                                        |
| Temperature               | kelvin          | K                  | Defined as the fraction 1/273.16 of the thermodynamic temperature of the triple point of water.                                                                                                                                                                                    |
| Time                      | second          | s                  | Duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium-133 atom.                                                                                                                    |
| 2. Supplementary SI units |                 |                    |                                                                                                                                                                                                                                                                                    |
| Plane angle               | radian          | rad                | The plane angle between two radii of a circle which cut off on the circumference an arc equal in length to the radius.                                                                                                                                                             |
| Solid angle               | steradian       | sr                 | The solid angle which, having its vertex in the center of a sphere, cuts off an area of the surface of the sphere equal to that of a square with sides of length equal to the radius of the sphere.                                                                                |

TABLE 2.1 Fundamental Physical Constants (Continued)

| B. Derived SI units                                    |                                  |                                                                   |                                                                                                                    |
|--------------------------------------------------------|----------------------------------|-------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|
| Physical quantity                                      | Name of SI unit                  | Symbol for SI unit                                                | Expression in terms of SI base units                                                                               |
| Absorbed dose (of radiation)                           | gray                             | Gy                                                                | $\text{J} \cdot \text{kg}^{-1}$                                                                                    |
| Activity (radioactive)                                 | becquerel                        | Bq                                                                | $\text{s}^{-1} = \text{m}^2 \cdot \text{s}^{-2}$                                                                   |
| Capacitance (electric)                                 | farad                            | F                                                                 | $\text{C} \cdot \text{V}^{-1} = \text{m}^{-2} \cdot \text{kg}^{-1} \cdot \text{s}^4 \cdot \text{A}^2$              |
| Charge (electric)                                      | coulomb                          | C                                                                 | $\text{A} \cdot \text{s}$                                                                                          |
| Conductance (electric)                                 | siemens                          | S                                                                 | $\Omega^{-1} = \text{m}^{-2} \cdot \text{kg}^{-1} \cdot \text{s}^3 \cdot \text{A}^2$                               |
| Dose equivalent (radiation)                            | sievert                          | Sv                                                                | $\text{J} \cdot \text{kg}^{-1} = \text{m}^2 \cdot \text{s}^{-2}$                                                   |
| Energy, work, heat                                     | joule                            | J                                                                 | $\text{N} \cdot \text{m} = \text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2}$                                         |
| Force                                                  | newton                           | N                                                                 | $\text{m} \cdot \text{kg} \cdot \text{s}^{-2}$                                                                     |
| Frequency                                              | hertz                            | Hz                                                                | $\text{s}^{-1}$                                                                                                    |
| Illuminance                                            | lux                              | lx                                                                | $\text{cd} \cdot \text{sr} \cdot \text{m}^{-2}$                                                                    |
| Inductance                                             | henry                            | H                                                                 | $\text{V} \cdot \text{A}^{-1} \cdot \text{s} = \text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-2}$ |
| Luminous flux                                          | lumen                            | Lm                                                                | $\text{cd} \cdot \text{sr}$                                                                                        |
| Magnetic flux                                          | weber                            | Wb                                                                | $\text{V} \cdot \text{s} = \text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-1}$                     |
| Magnetic flux density                                  | tesla                            | T                                                                 | $\text{V} \cdot \text{s} \cdot \text{m}^{-2} = \text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-1}$                  |
| Potential, electric<br>(electromotive force)           | volt                             | V                                                                 | $\text{J} \cdot \text{C}^{-1} = \text{m}^2 \cdot \text{kg} \cdot \text{s}^{-3} \cdot \text{A}^{-1}$                |
| Power, radiant flux                                    | watt                             | W                                                                 | $\text{J} \cdot \text{s}^{-1} = \text{m}^2 \cdot \text{kg} \cdot \text{s}^{-3}$                                    |
| Pressure, stress                                       | pascal                           | Pa                                                                | $\text{N} \cdot \text{m}^{-2} = \text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-2}$                                 |
| Resistance, electric                                   | ohm                              | $\Omega$                                                          | $\text{V} \cdot \text{A}^{-1} = \text{m}^2 \cdot \text{kg} \cdot \text{s}^{-3} \cdot \text{A}^{-2}$                |
| Temperature, Celsius                                   | degree Celsius                   | $^{\circ}\text{C}$                                                | $^{\circ}\text{C} = (\text{K} - 273.15)$                                                                           |
| C. Recommended consistent values of constants          |                                  |                                                                   |                                                                                                                    |
| Quantity                                               | Symbol                           | Value*                                                            |                                                                                                                    |
| Anomalous electron moment correction                   | $\mu_e - 1$                      | 0.001 159 615(15)                                                 |                                                                                                                    |
| Atomic mass constant                                   | $m_u = 1 \text{ u}$              | $1.660\,540\,2(10) \times 10^{-27} \text{ kg}$                    |                                                                                                                    |
| Avogadro constant                                      | $L, N_A$                         | $6.022\,136\,7(36) \times 10^{23} \text{ mol}^{-1}$               |                                                                                                                    |
| Bohr magneton ( $= eh/4\pi m_e$ )                      | $\mu_B$                          | $9.274\,015\,4(31) \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$ |                                                                                                                    |
| Bohr radius                                            | $a_0$                            | $5.291\,772\,49(24) \times 10^{-11} \text{ m}$                    |                                                                                                                    |
| Boltzmann constant                                     | $k$                              | $1.380\,658(12) \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$    |                                                                                                                    |
| Charge-to-mass ratio for electron                      | $e/m_e$                          | $1.758\,805(5) \times 10^{-11} \text{ C} \cdot \text{kg}^{-1}$    |                                                                                                                    |
| Compton wavelength of electron                         | $\lambda_c$                      | $2.426\,309(4) \times 10^{-12} \text{ m}$                         |                                                                                                                    |
| Compton wavelength of neutron                          | $\lambda_{c,n}$                  | $1.319\,591(2) \times 10^{-15} \text{ m}$                         |                                                                                                                    |
| Compton wavelength of proton                           | $\lambda_{c,p}$                  | $1.321\,410(2) \times 10^{-15} \text{ m}$                         |                                                                                                                    |
| Diamagnetic shielding factor, spherical water molecule | $1 + \sigma(\text{H}_2\text{O})$ | 1.000 025 64(7)                                                   |                                                                                                                    |
| Electron magnetic moment                               | $\mu_e$                          | $9.284\,770\,1(31) \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$ |                                                                                                                    |
| Electron radius (classical)                            | $r_e$                            | $2.817\,938(7) \times 10^{-15} \text{ m}$                         |                                                                                                                    |
| Electron rest mass                                     | $m_e$                            | $9.109\,389\,7(54) \times 10^{-31} \text{ kg}$                    |                                                                                                                    |
| Elementary charge                                      | $e$                              | $1.602\,177\,33(49) \times 10^{-19} \text{ C}$                    |                                                                                                                    |
| Energy equivalents:                                    |                                  |                                                                   |                                                                                                                    |
| 1 electron mass                                        |                                  | 0.511 003 4(14) MeV                                               |                                                                                                                    |
| 1 electronvolt                                         | 1 eV/k                           | $1.160\,450(36) \times 10^4 \text{ K}$                            |                                                                                                                    |
|                                                        | 1 eV/hc                          | $8.065\,479(21) \times 10^3 \text{ cm}^{-1}$                      |                                                                                                                    |
|                                                        | 1 eV/h                           | $2.417\,970(6) \times 10^{14} \text{ Hz}$                         |                                                                                                                    |
| 1 neutron mass                                         |                                  | 939.573 1(27) MeV                                                 |                                                                                                                    |
| 1 proton mass                                          |                                  | 938.279 6(27) MeV                                                 |                                                                                                                    |

\* The digits in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digits.

**TABLE 2.1** Fundamental Physical Constants (*Continued*)

| C. Recommended consistent values of constants ( <i>continued</i> )  |                  |                                                                                     |
|---------------------------------------------------------------------|------------------|-------------------------------------------------------------------------------------|
| Quantity                                                            | Symbol           | Value*                                                                              |
| 1 u                                                                 |                  | 931.501 6(26) MeV                                                                   |
| Faraday constant                                                    | $F$              | 96 485.309(29) C · mol <sup>-1</sup>                                                |
| Fine structure constant                                             | $\alpha$         | 0.007 297 353 08(33)                                                                |
|                                                                     | $\alpha^{-1}$    | 137.035 989 5(61)                                                                   |
| First radiation constant                                            | $c_1$            | $3.741\,774\,9(22) \times 10^{-16}$ W · m <sup>2</sup>                              |
| Gas constant                                                        | $R$              | 8.314 510(70) J · K <sup>-1</sup> · mol <sup>-1</sup>                               |
| $g$ factor (Lande) for free electron                                | $g_e$            | 2.002 319 304 386(20)                                                               |
| Gravitational constant                                              | $G$              | $6.672\,59(85) \times 10^{-11}$ m <sup>3</sup> · kg <sup>-1</sup> · s <sup>-2</sup> |
| Hartree energy                                                      | $E_h$            | $4.359\,748\,2(26) \times 10^{-18}$ J                                               |
| Josephson frequency-voltage ratio                                   |                  | $4.835\,939(13) \times 10^{14}$ Hz · V <sup>-1</sup>                                |
| Magnetic flux quantum                                               | $\Phi_0$         | $2.067\,851(5) \times 10^{-15}$ Wb                                                  |
| Magnetic moment of protons in water                                 | $\mu_p/\mu_B$    | $1.520\,993\,129(17) \times 10^{-3}$                                                |
| Molar volume, ideal gas, $p = 1$ bar,<br>$\theta = 0^\circ\text{C}$ |                  | 22.711 08(19) L · mol <sup>-1</sup>                                                 |
| Neutron rest mass                                                   | $m_n$            | $1.674\,928\,6(10) \times 10^{-27}$ kg                                              |
| Nuclear magneton                                                    | $\mu_N$          | $5.050\,786\,6(17) \times 10^{-27}$ J · T <sup>-1</sup>                             |
| Permeability of vacuum                                              | $\mu_0$          | $4\pi \times 10^{-7}$ H · m <sup>-1</sup> exactly                                   |
| Permittivity of vacuum                                              | $\epsilon_0$     | $8.854\,187\,816 \times 10^{-12}$ F · m <sup>-1</sup>                               |
|                                                                     | $\hbar = h/2\pi$ | $1.054\,572\,66(63) \times 10^{-34}$ J · s                                          |
| Planck constant                                                     | $h$              | $6.626\,075\,5(40) \times 10^{-34}$ J · s                                           |
| Proton magnetic moment                                              | $\mu_p$          | $1.410\,607\,61(47) \times 10^{-26}$ J · T <sup>-1</sup>                            |
| Proton magnetogyric ratio                                           | $\gamma_p$       | $2.675\,221\,28(81) \times 10^8$ s <sup>-1</sup> · T <sup>-1</sup>                  |
| Proton resonance frequency per field in H <sub>2</sub> O            | $\gamma'_p/2\pi$ | $42.576\,375(13)$ MHz · T <sup>-1</sup>                                             |
| Proton rest mass                                                    | $m_p$            | $1.672\,623\,1(10) \times 10^{-27}$ kg                                              |
| Quantum-charge ratio                                                | $h/e$            | $4.135\,701(11) \times 10^{-15}$ J · Hz <sup>-1</sup> · C <sup>-1</sup>             |
| Quantum of circulation                                              | $h/m_e$          | $7.273\,89(1) \times 10^{-4}$ J · s · kg <sup>-1</sup>                              |
| Ratio, electron-to-proton magnetic moments                          | $\mu_e/\mu_p$    | $6.582\,106\,88(7) \times 10^2$                                                     |
| Rydberg constant                                                    | $R_\infty$       | $1.097\,373\,153\,4(13) \times 10^7$ m <sup>-1</sup>                                |
| Second radiation constant                                           | $c_2$            | $1.438\,769(12) \times 10^{-2}$ m · K                                               |
| Speed of light in vacuum                                            | $c_0$            | 299 792 458 m · s <sup>-1</sup> exactly                                             |
| Standard acceleration of free fall                                  | $g_n$            | 9.806 65 m · s <sup>-2</sup> exactly                                                |
| Standard atmosphere                                                 | atm              | 101 325 Pa exactly                                                                  |
| Stefan-Boltzmann constant                                           | $\sigma$         | $5.670\,51(19) \times 10^{-8}$ W · m <sup>-2</sup> · K <sup>-4</sup>                |
| Thomson cross section                                               | $\sigma_e$       | $6.652\,448(33) \times 10^{-29}$ m <sup>2</sup>                                     |
| Wien displacement constant                                          | $b$              | 0.289 78(4) cm · K                                                                  |
| Zeeman splitting constant                                           | $\mu_B/hc$       | $4.668\,58(4) \times 10^{-5}$ cm <sup>-1</sup> · G <sup>-1</sup>                    |

D. Units in use together with SI units

| Physical quantity | Name of unit                                  | Symbol for unit            | Value in SI units                   |
|-------------------|-----------------------------------------------|----------------------------|-------------------------------------|
| Area              | barn                                          | b                          | 10 <sup>-28</sup> m                 |
| Energy            | electronvolt<br>megaelectronvolt <sup>1</sup> | eV ( $e \times V$ )<br>MeV | $\approx 1.60218 \times 10^{-19}$ J |
| Length            | ångström <sup>2</sup>                         | Å                          | 10 <sup>-10</sup> m; 0.1 nm         |
| Mass              | tonne                                         | t                          | 10 <sup>3</sup> kg; Mg              |

\*The digits in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digits.

<sup>1</sup> The term million electronvolts is frequently used in place of megaelectronvolts.

<sup>2</sup> The ångström and bar are approved for temporary use with SI units; however, they should not be introduced if not used at present.

TABLE 2.1 Fundamental Physical Constants (Continued)

| D. Units in use together with SI units (continued) |                          |                               |                                              |
|----------------------------------------------------|--------------------------|-------------------------------|----------------------------------------------|
| Physical quantity                                  | Name of unit             | Symbol for unit               | Value in SI units                            |
|                                                    | unified atomic mass unit | $u [= m_a(^{12}\text{C})/12]$ | $\approx 1.66054 \times 10^{-27} \text{ kg}$ |
|                                                    | dalton <sup>3</sup>      | Da                            |                                              |
| Plane angle                                        | degree                   | °                             | $(\pi/180) \text{ rad}$                      |
|                                                    | minute                   | '                             | $(\pi/10\,800) \text{ rad}$                  |
|                                                    | second                   | "                             | $(\pi/648\,000) \text{ rad}$                 |
| Pressure                                           | bar <sup>2</sup>         | bar                           | $10^5 \text{ Pa} = 10^5 \text{ N m}^{-2}$    |
| Time                                               | minute                   | min                           | 60 s                                         |
|                                                    | hour                     | h                             | 3600 s                                       |
|                                                    | day                      | d                             | 86 400 s                                     |
| Volume                                             | liter (litre)            | L, l                          | $\text{dm}^3 = 10^{-3} \text{ m}^3$          |
|                                                    | milliliter               | mL, ml                        | $\text{cm}^3 = 10^{-6} \text{ m}^3$          |

<sup>2</sup> The ångström and bar are approved for temporary use with SI units; however, they should not be introduced if not used at present.

<sup>3</sup> The name dalton and symbol Da have not been approved although they are often used for large molecules.

TABLE 2.2 Physical and Chemical Symbols and Definitions

Symbols separated by commas represent equivalent recommendations. Symbols for physical and chemical quantities should be printed in *italic* type. Subscripts and superscripts which are themselves symbols for physical quantities should be italicized; all others should be in Roman type. Vectors and matrices should be printed in boldface italic type, e.g., ***B***, ***b***. Symbols for units should be printed in Roman type and should remain unaltered in the plural, and should not be followed by a full stop except at the end of a sentence. References: International Union of Pure and Applied Chemistry, *Quantities, Units and Symbols in Physical Chemistry*, Blackwell, Oxford, 1988; “Manual of Symbols and Terminology for Physicochemical Quantities and Units,” *Pure Applied Chem.* **31**:577–638 (1972), **37**:499–516 (1974), **46**:71–90 (1976), **51**:1–41, 1213–1218 (1979); **53**:753–771 (1981), **54**:1239–1250 (1982), **55**:931–941 (1983); IUPAP-SUN, “Symbols, Units and Nomenclature in Physics,” *Physica* **93A**: 1–60 (1978).

| A. Atoms and molecules                |                                   |                                                 |                                                               |
|---------------------------------------|-----------------------------------|-------------------------------------------------|---------------------------------------------------------------|
| Name                                  | Symbol                            | SI unit                                         | Definition                                                    |
| Activity (radioactivity)              | <i>A</i>                          | Bq                                              | $A = -dN_B/dt$                                                |
| Atomic mass constant                  | $m_u$                             | kg                                              | $m_u = m_a(^{12}\text{C})/12$                                 |
| Bohr magneton                         | $\mu_B$                           | $\text{J} \cdot \text{T}^{-1}$                  | $\mu_B = eh/4\pi m_e$                                         |
| Bohr radius                           | $a_0$                             | m                                               | $a_0 = 2\epsilon_0 h^2/m_e e^2$                               |
| Decay (rate) constant                 | $\lambda$                         | $\text{s}^{-1}$                                 | $A = \lambda N_B$                                             |
| Dissociation energy                   | $D, E_d$                          | J                                               |                                                               |
|                                       | $D_0$                             | J                                               |                                                               |
| From ground state                     | $D_e$                             | J                                               |                                                               |
| From the potential minimum            |                                   |                                                 |                                                               |
| Electric dipole moment of a molecule  | <b><i>p</i></b> , <b><i>μ</i></b> | $\text{C} \cdot \text{m}$                       | $E_p = -\mathbf{p} \cdot \mathbf{E}$                          |
| Electric field gradient               | <b><i>q</i></b>                   | $\text{V} \cdot \text{m}^{-2}$                  | $q_{\alpha\beta} = -\partial^2 V/\partial\alpha\partial\beta$ |
| Electric polarizability of a molecule | $\alpha$                          | $\text{C} \cdot \text{m}^2 \cdot \text{V}^{-1}$ | $p(\text{induced}) = \alpha E$                                |
| Electron affinity                     | $E_{ea}$                          | J                                               |                                                               |
| Electron rest mass                    | $m_e$                             | kg                                              |                                                               |
| Elementary charge, proton charge      | <i>e</i>                          | C                                               |                                                               |
| Fine structure constant               | $\alpha$                          |                                                 | $\alpha = e^2/2\epsilon_0 hc$                                 |
| <i>g</i> factor                       | <i>g</i>                          |                                                 |                                                               |

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| A. Atoms and molecules (continued)                               |                                   |                                    |                                                                                           |
|------------------------------------------------------------------|-----------------------------------|------------------------------------|-------------------------------------------------------------------------------------------|
| Name                                                             | Symbol                            | SI unit                            | Definition                                                                                |
| Hartree energy                                                   | $E_h$                             | J                                  | $E_h = h^2/4\pi^2 m_e a_0^2$                                                              |
| Ionization energy                                                | $E_i$                             | J                                  |                                                                                           |
| Larmor circular frequency                                        | $\omega_L$                        | $s^{-1}$                           | $\omega_L = (e/2m)B$                                                                      |
| Larmor frequency                                                 | $\nu_L$                           | Hz                                 | $\nu_L = \omega_L/2\pi$                                                                   |
| Longitudinal relaxation time                                     | $T_1$                             | s                                  |                                                                                           |
| Magnetogyric ratio                                               | $\gamma$                          | $C \cdot kg^{-1}$                  | $\gamma = \mu/L$                                                                          |
| Magnetic dipole moment of a molecule                             | $\mathbf{m}, \boldsymbol{\mu}$    | $J \cdot T^{-1}$                   | $E_p = -\mathbf{m} \cdot \mathbf{B}$                                                      |
| Magnetizability of a molecule                                    | $\xi$                             | $J \cdot T^{-2}$                   | $\mathbf{m} = \xi \mathbf{B}$                                                             |
| Mass of atom, atomic mass                                        | $m, m_a$                          | kg                                 |                                                                                           |
| Neutron number                                                   | $N$                               |                                    | $N = A - Z$                                                                               |
| Nuclear magneton                                                 | $\mu_N$                           | $J \cdot T^{-1}$                   | $\mu_N = (m_e/m_p)\mu_B$                                                                  |
| Nucleon number, mass number                                      | $A$                               |                                    |                                                                                           |
| Planck constant                                                  | $h$                               | $J \cdot s$                        |                                                                                           |
| Planck constant/ $2\pi$                                          | $\hbar$                           | $J \cdot s$                        | $\hbar = h/2\pi$                                                                          |
| Principal quantum number (H atom)                                | $n$                               |                                    | $E = -hcR/n^2$                                                                            |
| Proton number, atomic number                                     | $Z$                               |                                    |                                                                                           |
| Quadrupole interaction                                           | $\chi$                            | J                                  | $\chi_{\alpha\beta} = eQq_{\alpha\beta}$                                                  |
| Quadrupole moment of a molecule                                  | $\mathbf{Q}; \boldsymbol{\Theta}$ | $C \cdot m^2$                      | $E_p = 0.5 \mathbf{Q} : \mathbf{V}''$<br>$= \frac{1}{3} \boldsymbol{\Theta} \mathbf{V}''$ |
| Quadrupole moment                                                | $eQ$                              | $C \cdot m^2$                      | $eQ = 2\langle \Theta_{zz} \rangle$                                                       |
| Rydberg constant                                                 | $R_\infty$                        | $m^{-1}$                           | $R_\infty = E_H/2hc$                                                                      |
| Transverse relaxation time                                       | $T_2$                             | s                                  |                                                                                           |
| B. Chemical reactions                                            |                                   |                                    |                                                                                           |
| Name                                                             | Symbol                            | SI unit                            | Definition                                                                                |
| Amount (of substance)                                            | $n$                               | mol                                | $n_B = N_B/L$                                                                             |
| Atomic mass                                                      | $m, m_a$                          | kg                                 |                                                                                           |
| Atomic mass constant <sup>a</sup>                                | $m_u$                             | kg                                 | $m_u = m_a(^{12}\text{C})/12$                                                             |
| Avogadro constant                                                | $L, N_A$                          | $\text{mol}^{-1}$                  |                                                                                           |
| Concentration, amount (concentration)                            | $c$                               | $\text{mol} \cdot \text{m}^{-3}$   | $c_B = n_B/V$                                                                             |
| Degree of dissociation                                           | $\alpha$                          |                                    |                                                                                           |
| Density (mass)                                                   | $\rho, \gamma$                    | $\text{kg} \cdot \text{m}^{-3}$    | $\rho = m_B/V$                                                                            |
| Extent of reaction, advancement                                  | $\xi$                             | mol                                | $\Delta\xi = \Delta n_B/\nu_{BB}$                                                         |
| Mass (molecular or formula unit)                                 | $m, m_i$                          | kg                                 |                                                                                           |
| Mass fraction                                                    | $w$                               |                                    | $w_B = m_B/\Sigma m_i$                                                                    |
| Molality (of a solute)                                           | $m$                               | $\text{mol} \cdot \text{kg}^{-1}$  | $m_B = n_B/m_A$                                                                           |
| Molar mass                                                       | $M$                               | $\text{kg} \cdot \text{mol}^{-1}$  | $M_B = m/n_B$                                                                             |
| Molar volume                                                     | $V_m$                             | $\text{m}^3 \cdot \text{mol}^{-1}$ | $V_{m,B} = V/n_B$                                                                         |
| Molecular weight (relative molar mass)                           | $M_r$                             |                                    | $M_{r,B} = m_B/m_u$                                                                       |
| Mole fraction <sup>b</sup> , number fraction                     | $x, y$                            |                                    | $x_B = n_B/\Sigma n_i$                                                                    |
| Number concentration                                             | $C, n$                            | $\text{m}^{-3}$                    | $C_B = N_B/V$                                                                             |
| Number of entities (e.g., molecules, atoms, ions, formula units) | $N$                               |                                    |                                                                                           |
| Pressure (partial)                                               | $p_B$                             | Pa                                 | $p_B = y_B p$                                                                             |
| Pressure (total)                                                 | $p, P$                            | Pa                                 |                                                                                           |
| Solubility                                                       | $s$                               | $\text{mol} \cdot \text{m}^{-3}$   | $s_B = c_B$ (saturated solution)                                                          |

<sup>a</sup> In biochemistry this unit is called the dalton, with symbol Da.  
<sup>b</sup> For condensed phases  $x$  is used, and for gaseous mixtures  $y$  may be used.

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| B. Chemical reactions ( <i>continued</i> )                                                                                  |                                       |                                                                    |                                   |                                             |
|-----------------------------------------------------------------------------------------------------------------------------|---------------------------------------|--------------------------------------------------------------------|-----------------------------------|---------------------------------------------|
| Name                                                                                                                        |                                       | Symbol                                                             | SI unit                           | Definition                                  |
| Stoichiometric number                                                                                                       |                                       | $\nu$                                                              |                                   |                                             |
| Surface concentration                                                                                                       |                                       | $\Gamma$                                                           | $\text{mol} \cdot \text{m}^{-2}$  | $\Gamma_{\text{B}} = n_{\text{B}}/A$        |
| Volume fraction                                                                                                             |                                       | $\phi$                                                             |                                   | $\phi_{\text{B}} = V_{\text{B}}/\Sigma V_i$ |
| Symbols for particles and nuclear reactions:                                                                                |                                       |                                                                    |                                   |                                             |
| Alpha particle                                                                                                              | $\alpha$                              | Muon, positive                                                     | $\mu^+$                           |                                             |
| Beta particle                                                                                                               | $\beta^-, \beta^+$                    | Neutron                                                            | n, $n^0$                          |                                             |
| Deuteron                                                                                                                    | d, ${}^2\text{H}$                     | Photon                                                             | $\gamma$                          |                                             |
| Electron                                                                                                                    | e, $e^-$                              | Proton                                                             | p, $p^+$                          |                                             |
| Helion                                                                                                                      | h                                     | Triton                                                             | t, ${}^3\text{H}$                 |                                             |
| Muon, negative                                                                                                              | $\mu^-$                               |                                                                    |                                   |                                             |
| The meaning of the symbolic expression indicating a nuclear reaction:                                                       |                                       |                                                                    |                                   |                                             |
| initial nuclide                                                                                                             |                                       | (incoming particles, outgoing particles)<br>(or quanta, or quanta) |                                   | final nuclide                               |
| <i>Examples:</i> ${}^{14}\text{N}(\alpha, \text{p}){}^{17}\text{O}$ , ${}^{23}\text{Na}(\gamma, 3\text{n}){}^{20}\text{Na}$ |                                       |                                                                    |                                   |                                             |
| States of aggregation:                                                                                                      |                                       |                                                                    |                                   |                                             |
| am                                                                                                                          | amorphous solid                       | cd                                                                 | condensed phase (solid or liquid) |                                             |
| aq                                                                                                                          | aqueous solution                      | cr                                                                 | crystalline                       |                                             |
| as, $\infty$                                                                                                                | aqueous solution at infinite dilution | fl                                                                 | fluid phase (gas or liquid)       |                                             |
|                                                                                                                             |                                       | lc                                                                 | liquid crystal                    |                                             |
| g                                                                                                                           | gas                                   | vit                                                                | vitreous substance                |                                             |
| l                                                                                                                           | liquid                                | mon                                                                | monomeric form                    |                                             |
| s                                                                                                                           | solid                                 | pol                                                                | polymeric form                    |                                             |
| sln                                                                                                                         | solution                              | ads                                                                | species adsorbed on a substance   |                                             |
| C. Chromatography                                                                                                           |                                       |                                                                    |                                   |                                             |
| Name                                                                                                                        |                                       | Symbol                                                             | Definition                        |                                             |
| Adjusted retention time                                                                                                     |                                       | $t'_R$                                                             | $t'_R = t_R - t_M$                |                                             |
| Adjusted retention volume                                                                                                   |                                       | $V'_R$                                                             | $V'_R = V_R - V_M$                |                                             |
| Average linear gas velocity                                                                                                 |                                       | $\mu$                                                              | $\mu = L/t_M$                     |                                             |
| Band variance                                                                                                               |                                       | $\sigma^2$                                                         |                                   |                                             |
| Bed volume                                                                                                                  |                                       | $V_g$                                                              |                                   |                                             |
| Capacity, volume                                                                                                            |                                       | $Q_v$                                                              |                                   |                                             |
| Capacity, weight                                                                                                            |                                       | $Q_w$                                                              |                                   |                                             |
| Column length                                                                                                               |                                       | $L$                                                                |                                   |                                             |
| Column temperature                                                                                                          |                                       | $\theta$                                                           |                                   |                                             |
| Column volume                                                                                                               |                                       | $V_{\text{col}}$                                                   | $V_{\text{col}} = \pi D_c^2/4$    |                                             |
| Concentration at peak maximum                                                                                               |                                       | $C_{\text{max}}$                                                   |                                   |                                             |
| Concentration of solute in mobile phase                                                                                     |                                       | $C_M$                                                              |                                   |                                             |
| Concentration of solute in stationary phase                                                                                 |                                       | $C_S$                                                              |                                   |                                             |
| Density of liquid phase                                                                                                     |                                       | $\rho_L$                                                           |                                   |                                             |
| Diffusion coefficient, liquid film                                                                                          |                                       | $D_f$                                                              |                                   |                                             |
| Diffusion coefficient, mobile phase                                                                                         |                                       | $D_M$                                                              |                                   |                                             |



**TABLE 2.2** Physical and Chemical Symbols and Definitions (*Continued*)

| C. Chromatography ( <i>continued</i> )   |                |                                                                                                                                             |
|------------------------------------------|----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Name                                     | Symbol         | Definition                                                                                                                                  |
| Diffusion coefficient, stationary phase  | $D_s$          |                                                                                                                                             |
| Distribution ratio                       | $D_c$          | $= [A^+]_s/[A^+]_m$<br>$= \frac{\text{amount of A per cm}^3 \text{ stationary phase}}{\text{amount of A per cm}^3 \text{ of mobile phase}}$ |
|                                          | $D_g$          | $= \frac{\text{amount A per gram dry stationary phase}}{\text{amount A per cm}^3 \text{ of mobile phase}}$                                  |
|                                          | $D_v$          | $= \frac{\text{amount A, stationary phase per cm}^3 \text{ bed volume}}{\text{amount A per cm}^3 \text{ of mobile phase}}$                  |
|                                          | $D_s$          | $= \frac{\text{amount of A per m}^2 \text{ of surface}}{\text{amount of A per cm}^3 \text{ of mobile phase}}$                               |
| Elution volume, exclusion chromatography | $V_e$          |                                                                                                                                             |
| Flow rate, column                        | $F_c$          | $F_c = (\pi d_c^2/4)(\epsilon_{tot})(L/t_M)$                                                                                                |
| Gas/liquid volume ratio                  | $\beta$        |                                                                                                                                             |
| Inner column volume                      | $V_i$          |                                                                                                                                             |
| Interstitial (outer) volume              | $V_o$          |                                                                                                                                             |
| Kovats retention indices                 | RI             |                                                                                                                                             |
| Matrix volume                            | $V_g$          |                                                                                                                                             |
| Net retention volume                     | $V_N$          | $V_N = jV'_R$                                                                                                                               |
| Obstruction factor                       | $\gamma$       |                                                                                                                                             |
| Packing uniformity factor                | $\lambda$      |                                                                                                                                             |
| Particle diameter                        | $d_p$          | $d_p = L/Nh$                                                                                                                                |
| Partition coefficient                    | $K$            | $K = C_s/C_m = (V_R - V_M)/V_s$                                                                                                             |
| Partition ratio                          | $k'$           | $k' = C_s V_s / C_m V_M = K(V_s/V_M)$                                                                                                       |
| Peak asymmetry factor                    | AF             | Ratio of peak half-widths at 10% peak height                                                                                                |
| Peak resolution                          | Rs             | $Rs = (t_{R,2} - t_{R,1})/0.5(W_2 + W_1)$                                                                                                   |
| Plate height                             | $H$            | $H = L/N_{eff}$                                                                                                                             |
| Plate number                             | $N_{eff}$      | $N_{eff} = L/H = 16(t'_R/W_b)^2 = 5.54(t'_R/W_{1/2})^2$                                                                                     |
| Porosity, column                         | $\epsilon$     |                                                                                                                                             |
| Pressure, column inlet                   | $p_i$          |                                                                                                                                             |
| Pressure, column outlet                  | $p_o$          |                                                                                                                                             |
| Pressure drop                            | $\Delta P$     |                                                                                                                                             |
| Pressure-gradient correction             | $j$            | $j = \frac{3[(p_i/p_o)^2 - 1]}{2[(p_i/p_o)^3 - 1]}$                                                                                         |
| Recovery factor                          | $R_n$          | $R_n = 1 - (rD_c + 1)^{-n}$ ; $r = V_{org}/V_{aq}$                                                                                          |
| Reduced column length                    | $\lambda$      | $\lambda = L/d_p$                                                                                                                           |
| Reduced plate height                     | $h$            | $h = H/d_p$                                                                                                                                 |
| Reduced velocity                         | $v$            | $v = \mu d_p / D_M = K d_p / t_M D_M$                                                                                                       |
| Relative retention ratio                 | $\alpha$       | $\alpha = (k'_2/k'_1)$                                                                                                                      |
| Retardation factor <sup>c</sup>          | $R_f$          | $R_f = d_{solute}/d_{mobile \text{ phase}}$                                                                                                 |
| Retention time                           | $t_R$          | $t_R = t_M(1 + k') = L/\mu$                                                                                                                 |
| Retention volume                         | $V_R$          | $V_R = t_R F_c$                                                                                                                             |
| Selectivity coefficient <sup>d</sup>     | $k_{A,B}$      | $k_{A,B} = [A^+]_i[B^+]_i/[B^+]_i[A^+]_i$                                                                                                   |
| Separation factor                        | $\alpha_{A/B}$ | $\alpha_{A/B} = (D_c)_A/(D_c)_B$                                                                                                            |

<sup>c</sup> The distance  $d$  corresponds to the movement of solute and mobile phase from the starting (sample spotting) line.<sup>d</sup> Subscript "i" represents an ion-exchange resin phase. Two immiscible liquid phases might be represented similarly using subscripts "1" and "2."

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| C. Chromatography (continued)               |                   |                                                  |                                             |
|---------------------------------------------|-------------------|--------------------------------------------------|---------------------------------------------|
| Name                                        | Symbol            | Definition                                       |                                             |
| Specific retention volume                   | $V_g^\circ$       | $V_g^\circ = 273\text{ }R/(p^\circ\text{ }Mw_L)$ |                                             |
| Thickness (effective) of stationary phase   | $d_f$             |                                                  |                                             |
| Total bed volume                            | $V_{\text{tot}}$  |                                                  |                                             |
| Transit time of nonretained solute          | $t_M, t_0$        |                                                  |                                             |
| Vapor pressure                              | $p$               |                                                  |                                             |
| Volume liquid phase in column               | $V_L$             |                                                  |                                             |
| Volume mobile phase in column               | $V_M$             |                                                  |                                             |
| Weight of liquid phase                      | $w_L$             |                                                  |                                             |
| Zone width at baseline                      | $W_b$             | $W_b = 4\sigma$                                  |                                             |
| Zone width at $\frac{1}{2}$ peak height     | $W_{1/2}$         |                                                  |                                             |
| D. Colloid and surface chemistry            |                   |                                                  |                                             |
| Name                                        | Symbol            | SI unit                                          | Definition                                  |
| Adsorbed amount of B                        | $n_B^s$           | mol                                              |                                             |
| Area per molecule                           | $a, \sigma$       | $\text{m}^2$                                     | $a_B = A/N_N^\sigma$                        |
| Area per molecule in a filled monolayer     | $a_m$             | $\text{m}^2$                                     | $a_{m,B} = A/N_{m,B}$                       |
| Average molar masses:                       |                   |                                                  |                                             |
| Mass-average                                | $M_m$             | $\text{kg} \cdot \text{mol}^{-1}$                | $M_m = \Sigma n_i M_i^2 / \Sigma n_i M_i$   |
| Number-average                              | $M_n$             | $\text{kg} \cdot \text{mol}^{-1}$                | $M_n = \Sigma n_i M_i / \Sigma n_i$         |
| Z-average                                   | $M_Z$             | $\text{kg} \cdot \text{mol}^{-1}$                | $M_Z = \Sigma n_i M_i^3 / \Sigma n_i M_i^2$ |
| Contact angle                               | $\theta$          | rad                                              |                                             |
| Film tension                                | $\Sigma_f$        | $\text{N} \cdot \text{m}^{-1}$                   | $\Sigma_f = 2\gamma_f$                      |
| Film thickness                              | $t, h, \delta$    | m                                                |                                             |
| Reciprocal thickness of the double layer    | $\kappa$          | $\text{m}^{-1}$                                  | $\kappa = [2F^2 I_c / \epsilon RT]^{1/2}$   |
| Retarded van der Waals constant             | $\beta, B$        | J                                                |                                             |
| Sedimentation coefficient <sup>e</sup>      | $s$               | s                                                | $s = v/a$                                   |
| Specific surface area                       | $a, s, a_s$       | $\text{m}^2/\text{kg}$                           | $a = A/m$                                   |
| Surface coverage                            | $\theta$          |                                                  | $\theta = N_B^\sigma/N_B$                   |
| Surface excess of B                         | $n_B^g$           | mol                                              |                                             |
| Surface pressure                            | $\pi^s, \pi$      | $\text{N} \cdot \text{m}^{-1}$                   | $\pi^s = \gamma^0 - \gamma$                 |
| Surface tension, interfacial tension        | $\gamma, \sigma$  | $\text{J} \cdot \text{m}^{-2}$                   | $\gamma = (\partial G/\partial A_s)_{T,p}$  |
| Thickness of (surface or interfacial) layer | $\tau, \delta, t$ | m                                                |                                             |
| Total surface excess concentration          | $\Gamma$          | $\text{mol} \cdot \text{m}^{-2}$                 | $\Gamma = \Sigma \Gamma_i$                  |
| van der Waals constant                      | $\lambda$         | J                                                |                                             |
| van der Waals-Hamaker constant              | $A_H$             | J                                                |                                             |

<sup>e</sup>  $v$  is the velocity of sedimentation and  $a$  is the acceleration of free fall or centrifugation.

**TABLE 2.2** Physical and Chemical Symbols and Definitions (*Continued*)

| E. Electricity and magnetism                       |                                |                     |                                                   |
|----------------------------------------------------|--------------------------------|---------------------|---------------------------------------------------|
| Name                                               | Symbol                         | SI unit             | Definition                                        |
| Admittance                                         | $Y$                            | S                   | $Y = 1/Z$                                         |
| Capacitance                                        | $C$                            | F, $C \cdot V^{-1}$ | $C = Q/U$                                         |
| Charge density                                     | $\rho$                         | $C \cdot m^{-3}$    | $\rho = Q/V$                                      |
| Conductance                                        | $G$                            | S                   | $G = 1/R$                                         |
| Conductivity                                       | $\kappa$                       | $S \cdot m^{-1}$    | $\kappa = 1/\rho$                                 |
| Dielectric polarization (dipole moment per volume) | $\mathbf{P}$                   | $C \cdot m^{-2}$    | $\mathbf{P} = \mathbf{D} - \epsilon_0 \mathbf{E}$ |
| Electrical resistance                              | $R$                            | $\Omega$            | $R = U/I = \Delta V/I$                            |
| Electric current                                   | $I$                            | A                   | $I = dQ/dt$                                       |
| Electric current density                           | $j, \mathbf{J}$                | $A \cdot m^{-2}$    | $I = \int j \, dA$                                |
| Electric dipole moment                             | $\mathbf{p}, \boldsymbol{\mu}$ | $C \cdot m$         | $\mathbf{p} = \mathbf{Qr}$                        |
| Electric displacement                              | $\mathbf{D}$                   | $C \cdot m^{-2}$    | $\mathbf{D} = \epsilon \mathbf{E}$                |
| Electric field strength                            | $\mathbf{E}$                   | $V \cdot m^{-1}$    | $\mathbf{E} = \mathbf{F}/Q = -\text{grad } V$     |
| Electric flux                                      | $\Psi$                         | C                   | $\Psi = \int \mathbf{D} \, dA$                    |
| Electric potential                                 | $V, \phi$                      | V, $J \cdot C^{-1}$ | $V = dW/dQ$                                       |
| Electric potential difference                      | $U, \Delta V$                  | V                   | $U = V_2 - V_1$                                   |
| Electric susceptibility                            | $\chi_e$                       |                     | $\chi_e = \epsilon_r - 1$                         |
| Electromotive force                                | $E$                            | V                   | $E = \int (F/Q) \, ds$                            |
| Impedance                                          | $Z$                            | $\Omega$            | $Z = R + iX$                                      |
| Loss angle <sup>f</sup>                            | $\delta$                       | rad                 | $\delta = (\pi/2) + \phi_I - \phi_U$              |
| Magnetic dipole moment                             | $\mathbf{m}, \boldsymbol{\mu}$ | $A \cdot m^2$       | $E_p = -\mathbf{mB}$                              |
| Magnetic field strength                            | $\mathbf{H}$                   | $A \cdot m^{-1}$    | $\mathbf{B} = \mu \mathbf{H}$                     |
| Magnetic flux                                      | $\Phi$                         | Wb                  | $\Phi = \int \mathbf{B} \, dA$                    |
| Magnetization (magnetic dipole moment per volume)  | $\mathbf{M}$                   | $A \cdot m^{-1}$    | $\mathbf{M} = (\mathbf{B}/\mu_0) - \mathbf{H}$    |
| Magnetic susceptibility                            | $\chi, \kappa$                 |                     | $\chi = \mu_r - 1$                                |
| Magnetic vector potential                          | $\mathbf{A}$                   | $Wb \cdot m^{-1}$   | $\mathbf{B} = \nabla \mathbf{A}$                  |
| Molar magnetic susceptibility                      | $\chi_m$                       | $m^3/mol$           | $\chi_m = V_m \chi$                               |
| Mutual inductance                                  | $M, L_{12}$                    | H                   | $E_1 = L_{12}(dI_2/dt)$                           |
| Permeability                                       | $\mu$                          | $H \cdot m^{-1}$    | $\mathbf{B} = \mu \mathbf{H}$                     |
| Permeability of vacuum                             | $\mu_0$                        | $H \cdot m^{-1}$    |                                                   |
| Permittivity                                       | $\epsilon$                     | $F \cdot m^{-1}$    | $\mathbf{D} = \epsilon \mathbf{E}$                |
| Permittivity of vacuum                             | $\epsilon_0$                   | $F \cdot m^{-1}$    | $\epsilon_0 = \mu_0^{-1} c_0^{-2}$                |
| Poynting vector                                    | $\mathbf{S}$                   | $W \cdot m^{-2}$    | $\mathbf{S} = \mathbf{E} \cdot \mathbf{H}$        |
| Quantity of electricity, electric charge           | $Q$                            | C                   |                                                   |
| Reactance                                          | $X$                            | $\Omega$            | $X = (U/I) \sin \delta$                           |
| Relative permeability                              | $\mu_r$                        |                     | $\mu_r = \mu/\mu_0$                               |
| Relative permittivity <sup>g</sup>                 | $\epsilon_r$                   |                     | $\epsilon_r = \epsilon/\epsilon_0$                |
| Resistivity                                        | $\rho$                         | $\Omega \cdot m$    | $\rho = E/j$                                      |
| Self-inductance                                    | $L$                            | H                   | $E = -L(dI/dt)$                                   |
| Susceptance                                        | $B$                            | S                   | $Y = G + iB$                                      |

<sup>f</sup>  $\phi_I$  and  $\phi_U$  are the phases of current and potential difference.

<sup>g</sup> This quantity was formerly called the dielectric constant.

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| F. Electrochemistry                                               |                   |                                                      |                                                                                                |
|-------------------------------------------------------------------|-------------------|------------------------------------------------------|------------------------------------------------------------------------------------------------|
| Name                                                              | Symbol            | SI unit                                              | Definition                                                                                     |
| Charge density (surface)                                          | $\sigma$          | $\text{C} \cdot \text{m}^{-2}$                       | $\sigma = Q/A$                                                                                 |
| Charge number of an ion                                           | $z$               |                                                      | $z_{\text{B}} = Q_{\text{B}}/e$                                                                |
| Charge number of electrochemical cell reaction                    | $n, (z)$          |                                                      |                                                                                                |
| Conductivity (specific conductance)                               | $\kappa$          | $\text{S} \cdot \text{m}^{-1}$                       | $\kappa = j/E$                                                                                 |
| Conductivity cell constant                                        | $K_{\text{cell}}$ | $\text{m}^{-1}$                                      | $K_{\text{cell}} = \kappa R$                                                                   |
| Current density (electric)                                        | $j$               | $\text{A} \cdot \text{m}^{-2}$                       | $j = I/A$                                                                                      |
| Diffusion rate constant, mass transfer coefficient                | $k_{\text{d}}$    | $\text{m} \cdot \text{s}^{-1}$                       | $k_{\text{d,B}} =  \nu_{\text{B}} I_{1,\text{B}}/nF cA$                                        |
| Electric current                                                  | $I$               | A                                                    | $I = dQ/dt$                                                                                    |
| Electric mobility                                                 | $\mu$             | $\text{m}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$ | $\mu_{\text{B}} = v_{\text{B}}/E$                                                              |
| Electric potential difference (of a galvanic cell)                | $\Delta V, E, U$  | V                                                    | $\Delta V = V_{\text{R}} - V_{\text{L}}$                                                       |
| Electrochemical potential                                         | $\tilde{\mu}$     | $\text{J} \cdot \text{mol}^{-1}$                     | $\tilde{\mu}_{\text{B}}^{\alpha} = (\partial G / \partial n_{\text{B}}^{\alpha})$              |
| Electrode reaction rate constant                                  | $k$               | (varies)                                             | $k_{\text{ox}} = I_{\text{a}} / \left( nFA \prod_i c_i^{\eta_i} \right)$                       |
| Electrokinetic potential (zeta potential)                         | $\zeta$           | V                                                    |                                                                                                |
| Elementary charge (proton charge)                                 | $e$               | C                                                    |                                                                                                |
| emf, electromotive force                                          | $E$               | V                                                    | $E = \lim_{I \rightarrow 0} \Delta V$                                                          |
| emf of the cell                                                   | $E$               | V                                                    | $E = E^{\circ} - (RT/nF) \times \sum \nu_i \ln a_i$                                            |
| Faraday constant                                                  | $F$               | $\text{C} \cdot \text{mol}^{-1}$                     | $F = eL$                                                                                       |
| Galvani potential difference                                      | $\Delta \phi$     | V                                                    | $\Delta_{\alpha}^{\beta} \phi = \phi^{\beta} - \phi^{\alpha}$                                  |
| Inner electrode potential                                         | $\phi$            | V                                                    | $\nabla \phi = -E$                                                                             |
| Ionic conductivity                                                | $\lambda$         | $\text{S} \cdot \text{m}^2 \cdot \text{mol}^{-1}$    | $\lambda_{\text{B}} =  z_{\text{B}} Fu_{\text{B}}$                                             |
| Ionic strength                                                    | $I_{\text{c}}, I$ | $\text{mol} \cdot \text{m}^{-3}$                     | $I_{\text{c}} = \frac{1}{2} \sum c_i z_i^2$                                                    |
| Mean ionic activity                                               | $a_{\pm}$         |                                                      | $a_{\pm} = m_{\pm \gamma \pm} / m^0$                                                           |
| Mean ionic activity coefficient                                   | $\gamma_{\pm}$    |                                                      | $\gamma_{\pm}^{(\nu_+ + \nu_-)} = (\gamma_{\pm}^{\nu_+})(\gamma_{\pm}^{\nu_-})$                |
| Mean ionic mobility                                               | $m_{\pm}$         | $\text{mol} \cdot \text{kg}^{-1}$                    | $m_{\pm}^{(\nu_+ + \nu_-)} = (m_{\pm}^{\nu_+})(m_{\pm}^{\nu_-})$                               |
| Molar conductivity (of an electrolyte)                            | $\Lambda$         | $\text{S} \cdot \text{m}^{-2} \text{mol}^{-1}$       | $\Lambda_{\text{B}} = \kappa c_{\text{B}}$                                                     |
| pH                                                                | pH                |                                                      | $\text{pH} \approx -\log \left[ \frac{c(\text{H}^+)}{\text{mol} \cdot \text{dm}^{-3}} \right]$ |
| Outer electrode potential                                         | $\psi$            | V                                                    | $\psi = Q/4\pi\epsilon_0 r$                                                                    |
| Overpotential                                                     | $\eta$            | V                                                    | $\eta = E_{\text{I}} - E_{\text{I}=0} - IR_{\text{u}}$                                         |
| Reciprocal radius of ionic atmosphere                             | $\kappa$          | $\text{m}^{-1}$                                      | $\kappa = (2F^2 I / \epsilon RT)^{1/2}$                                                        |
| Standard emf, standard potential of electrochemical cell reaction | $E^0$             | V                                                    | $E^0 = -\Delta_{\text{c}} G^0 / nF = (RT/nF) \ln K$                                            |
| Surface electric potential                                        | $\chi$            | V                                                    | $\chi = \phi - \psi$                                                                           |
| Thickness diffusion layer                                         | $\delta$          | m                                                    | $\delta_{\text{B}} = D_{\text{B}}/k_{\text{d,B}}$                                              |
| Transfer coefficient                                              | $\alpha$          |                                                      | $\alpha_{\text{c}} = \frac{- \nu RT}{nF} \frac{\partial \ln  I_{\text{c}} }{\partial E}$       |
| Transport number                                                  | $t$               |                                                      | $t_{\text{B}} = j_{\text{B}} / \sum j_i$                                                       |
| Volta potential difference                                        | $\Delta \psi$     | V                                                    | $\Delta_{\alpha}^{\beta} = \psi^{\beta} - \psi^{\alpha}$                                       |

**TABLE 2.2** Physical and Chemical Symbols and Definitions (*Continued*)

| G. Electromagnetic radiation ( <i>continued</i> ) |                                       |                                                     |                                                           |
|---------------------------------------------------|---------------------------------------|-----------------------------------------------------|-----------------------------------------------------------|
| Name                                              | Symbol                                | SI unit                                             | Definition                                                |
| Absorbance                                        | $\alpha$                              |                                                     | $\alpha = \Phi_{\text{abs}}/\Phi_0$                       |
| Absorbance (decaidic)                             | $A$                                   |                                                     | $A = -\log(1 - \alpha_i)$                                 |
| Absorbance (napierian)                            | $B$                                   |                                                     | $B = -\ln(1 - \alpha_i)$                                  |
| Absorption coefficient:                           |                                       |                                                     |                                                           |
| Linear (decaidic)                                 | $a, K$                                | $\text{m}^{-1}$                                     | $a = A/l$                                                 |
| Linear (napierian)                                | $\alpha$                              | $\text{m}^{-1}$                                     | $\alpha = B/l$                                            |
| Molar (decaidic)                                  | $\epsilon$                            | $\text{m}^2 \cdot \text{mol}^{-1}$                  | $\epsilon = a/d = A/cl$                                   |
| Molar (napierian)                                 | $\kappa$                              | $\text{m}^2 \cdot \text{mol}^{-1}$                  | $\kappa = \alpha/c = B/cl$                                |
| Absorption index                                  | $k$                                   |                                                     | $k = \alpha/4\pi\tilde{\nu}$                              |
| Angle of optical rotation                         | $\alpha$                              | rad                                                 |                                                           |
| Circular frequency                                | $\omega$                              | $\text{s}^{-1}, \text{rad} \cdot \text{s}^{-1}$     | $\omega = 2\pi\nu$                                        |
| Complex refractive index                          | $\hat{n}$                             |                                                     | $\hat{n} = \eta + ik$                                     |
| Concentration, amount of substance                | $c$                                   | $\text{mol} \cdot \text{m}^3$                       |                                                           |
| Concentration, mass                               | $\gamma$                              | $\text{kg} \cdot \text{m}^3$                        |                                                           |
| Einstein transition probabilities:                |                                       |                                                     |                                                           |
| Spontaneous emission                              | $A_{nm}$                              | $\text{s}^{-1}$                                     | $dN_n/dt = -A_{nm}N_n$                                    |
| Stimulated absorption                             | $B_{mn}$                              | $\text{s} \cdot \text{kg}^{-1}$                     | $dN_n/dt = \rho_{\tilde{\nu}}(\tilde{\nu}_{nm})B_{mn}N_m$ |
| Stimulated emission                               | $B_{nm}$                              | $\text{s} \cdot \text{kg}^{-1}$                     | $dN_n/dt = \rho\tilde{\nu}(\tilde{\nu}_{nm})B_{mn}N_m$    |
| Emittance                                         | $\epsilon$                            |                                                     | $\epsilon = M/M_{\text{bb}}$                              |
| By blackbody                                      | $M_{\text{bb}}$                       |                                                     |                                                           |
| First radiation constant                          | $c_1$                                 | $\text{W} \cdot \text{m}^2$                         | $c_1 = 2\pi\hbar c_0^2$                                   |
| Frequency                                         | $\nu$                                 | Hz                                                  | $\nu = c/\lambda$                                         |
| Irradiance (radiant flux received)                | $E, (I)$                              | $\text{W} \cdot \text{m}^{-2}$                      | $E = d\Phi/dA$                                            |
| Molar refraction                                  | $R, R_m$                              | $\text{m}^3 \cdot \text{mol}^{-1}$                  | $R = \frac{(n^2 - 1)}{(n^2 + 2)} V_m$                     |
| Path length (absorbing)                           | $l$                                   | m                                                   |                                                           |
| Optical rotatory power                            | $[\alpha]_{\lambda}^{\theta}$         | rad                                                 | $[\alpha]_{\lambda}^{\theta} = \alpha/\gamma l$           |
| Planck constant                                   | $h$                                   | $\text{J} \cdot \text{s}$                           |                                                           |
| Planck constant/ $2\pi$                           | $\hbar$                               | $\text{J} \cdot \text{s}$                           | $\hbar = h/2\pi$                                          |
| Radiant energy                                    | $Q, W$                                | J                                                   |                                                           |
| Radiant energy density                            | $\rho, w$                             | $\text{J} \cdot \text{m}^{-3}$                      | $\rho = Q/V$                                              |
| Radiant exitance, emitted radiant flux            | $M$                                   | $\text{W} \cdot \text{m}^{-2}$                      | $M = d\Phi/dA_{\text{source}}$                            |
| Radiant intensity                                 | $I$                                   | $\text{W} \cdot \text{sr}^{-1}$                     | $I = d\Phi/d\Omega$                                       |
| Radiant power, radiant energy per time            | $\Phi, P$                             | W                                                   | $\Phi = dQ/dt$                                            |
| Refractive index                                  | $n$                                   |                                                     | $n = c_0/c$                                               |
| Reflectance                                       | $\rho$                                |                                                     | $\rho = \Phi_{\text{refl}}/\Phi_0$                        |
| Second radiation constant                         | $c_2$                                 | $\text{K} \cdot \text{m}$                           | $c_2 = \hbar c_0/k$                                       |
| Spectral radiant energy density:                  |                                       |                                                     |                                                           |
| In terms of frequency                             | $\rho_{\nu}, w_{\nu}$                 | $\text{J} \cdot \text{m}^{-3} \cdot \text{Hz}^{-1}$ | $\rho_{\nu} = d\rho/d\nu$                                 |
| In terms of wavelength                            | $\rho_{\lambda}, w_{\lambda}$         | $\text{J} \cdot \text{m}^{-4}$                      | $\rho_{\lambda} = d\rho/d\lambda$                         |
| In terms of wavenumber                            | $\rho_{\tilde{\nu}}, w_{\tilde{\nu}}$ | $\text{J} \cdot \text{m}^{-2}$                      | $\rho_{\tilde{\nu}} = d\rho/d\tilde{\nu}$                 |

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| G. Electromagnetic radiation (continued)           |                                |                                                                |                                                                  |
|----------------------------------------------------|--------------------------------|----------------------------------------------------------------|------------------------------------------------------------------|
| Name                                               | Symbol                         | SI unit                                                        | Definition                                                       |
| Speed of light:                                    |                                |                                                                |                                                                  |
| In a medium                                        | $c$                            | $\text{m} \cdot \text{s}^{-1}$                                 | $c = c_0/n$                                                      |
| In vacuum                                          | $c_0$                          | $\text{m} \cdot \text{s}^{-1}$                                 |                                                                  |
| Stefan-Boltzmann constant                          | $\sigma$                       | $\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$             | $M_{\text{bb}} = \sigma T^4$                                     |
| Transmittance                                      | $\tau, T$                      |                                                                | $\tau = \Phi_{\text{tr}}/\Phi_0$                                 |
| Wavelength                                         | $\lambda$                      | m                                                              |                                                                  |
| Wavenumber:                                        |                                |                                                                |                                                                  |
| In a medium                                        | $\sigma$                       | $\text{m}^{-1}$                                                | $\sigma = 1/\lambda$                                             |
| In vacuum                                          | $\tilde{\nu}$                  | $\text{m}^{-1}$                                                | $\tilde{\nu} = \nu/c_0 = 1/n\lambda$                             |
| H. Kinetics                                        |                                |                                                                |                                                                  |
| Name                                               | Symbol                         | SI unit                                                        | Definition                                                       |
| Activation energy                                  | $E_{\text{a}}, E$              | $\text{J} \cdot \text{mol}^{-1}$                               | $E_{\text{a}} = RT^2 d \ln k/dT$                                 |
| Boltzmann constant                                 | $k, k_{\text{B}}$              | $\text{J} \cdot \text{K}^{-1}$                                 |                                                                  |
| Collision cross section                            | $\sigma$                       | $\text{m}^2$                                                   | $\sigma_{\text{AB}} = \pi d_{\text{AB}}^2$                       |
| Collision diameter                                 | $d$                            | m                                                              | $d_{\text{AB}} = r_{\text{A}} + r_{\text{B}}$                    |
| Collision frequency                                | $Z_{\text{A}}$                 | $\text{s}^{-1}$                                                |                                                                  |
| Collision frequency factor                         | $z_{\text{AB}}, z_{\text{AA}}$ | $\text{m}^3 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$         | $z_{\text{AB}} = Z_{\text{AB}}/Lc_{\text{A}}c_{\text{B}}$        |
| Collision number                                   | $Z_{\text{AB}}, Z_{\text{AA}}$ | $\text{m}^{-3} \cdot \text{s}^{-1}$                            |                                                                  |
| Half-life                                          | $t_{1/2}$                      | s                                                              | $c(t_{1/2}) = c_0/2$                                             |
| Overall order of reaction                          | $n$                            |                                                                | $n = \sum n_{\text{B}}$                                          |
| Partial order of reaction                          | $n_{\text{B}}$                 |                                                                | $\nu = k\Pi c_{\text{B}}^{\nu_{\text{B}}}$                       |
| Pre-exponential factor                             | $A$                            | $(\text{mol}^{-1} \cdot \text{m}^3)^{n-1} \cdot \text{s}^{-1}$ | $k = A \exp(-E_{\text{a}}/RT)$                                   |
| Quantum yield, photochemical yield                 | $\phi$                         |                                                                |                                                                  |
| Rate of change of quantity $X$                     | $\dot{X}$                      | (varies)                                                       | $\dot{X} = dX/dt$                                                |
| Rate of concentration change (chemical reaction)   | $r_{\text{B}}, \nu_{\text{B}}$ | $\text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$           | $r_{\text{B}} = dc_{\text{B}}/dt$                                |
| Rate constant, rate coefficient                    | $k$                            | $(\text{mol}^{-1} \cdot \text{m}^3)^{n-1} \cdot \text{s}^{-1}$ | $\nu = k\Pi c_{\text{B}}^{\nu_{\text{B}}}$                       |
| Rate of conversion change due to chemical reaction | $\dot{\zeta}$                  | $\text{mol} \cdot \text{s}^{-1}$                               | $\dot{\zeta} = d\zeta/dt$                                        |
| Rate of reaction (based on concentration)          | $\nu$                          | $\text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$           | $\nu = \zeta/V = \nu_{\text{B}}^{-1} dc_{\text{B}}/dt$           |
| Relaxation time                                    | $\tau$                         | s                                                              | $\tau = 1/(k_1 + k_{-1})$                                        |
| Standard enthalpy of activation                    | $\Delta H_{\ddagger}^{\circ}$  | $\text{J} \cdot \text{mol}^{-1}$                               |                                                                  |
| Standard entropy of activation                     | $\Delta S_{\ddagger}^{\circ}$  | $\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$           |                                                                  |
| Standard Gibbs energy of activation                | $\Delta G_{\ddagger}^{\circ}$  | $\text{J} \cdot \text{mol}^{-1}$                               |                                                                  |
| Volume of activation                               | $\Delta_{\ddagger}^{\circ}V$   | $\text{m}^3 \cdot \text{mol}^{-1}$                             | $\Delta_{\ddagger}^{\circ}V = -RT (\partial \ln k/\partial p)_T$ |

**TABLE 2.2** Physical and Chemical Symbols and Definitions (*Continued*)

| I. Mechanics                           |                            |                                                              |                                             |
|----------------------------------------|----------------------------|--------------------------------------------------------------|---------------------------------------------|
| Name                                   | Symbol                     | SI unit                                                      | Definition                                  |
| Acoustic factors:                      |                            |                                                              |                                             |
| Absorption                             | $\alpha_a$                 |                                                              | $\alpha_a = 1 - \rho$                       |
| Dissipation                            | $\delta$                   |                                                              | $\delta = \alpha_a - \tau$                  |
| Reflection                             | $\rho$                     |                                                              | $\rho = P_r/P_0$                            |
| Transmission                           | $\tau$                     |                                                              | $\tau = P_t/P_0$                            |
| Angular momentum                       | $\mathbf{L}$               | $\text{J} \cdot \text{s}$                                    | $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ |
| Bulk modulus, compression modulus      | $K$                        | Pa                                                           | $K = -V_0(dp/dV)$                           |
| Density, mass density                  | $\rho$                     | $\text{kg} \cdot \text{m}^{-3}$                              | $\rho = m/V$                                |
| Energy                                 | $E$                        | J                                                            |                                             |
| Fluidity, kinematic viscosity          | $\phi$                     | $\text{m} \cdot \text{kg}^{-1} \cdot \text{s}$               | $\phi = 1/\eta$                             |
| Force                                  | $\mathbf{F}$               | N                                                            | $\mathbf{F} = d\mathbf{p}/dt = m\mathbf{a}$ |
| Friction coefficient                   | $\mu, (f)$                 |                                                              | $F_{\text{frict}} = \mu F_{\text{norm}}$    |
| Gravitational constant                 | $G$                        | $\text{N} \cdot \text{m}^2 \cdot \text{kg}^{-2}$             | $F = Gm_1m_2/r^2$                           |
| Hamilton function                      | $H$                        | J                                                            | $H(q, p) = T(q, p) + V(q)$                  |
| Kinematic viscosity                    | $\nu$                      | $\text{m}^2 \cdot \text{s}^{-1}$                             | $\nu = \eta/\rho$                           |
| Kinetic energy                         | $E_k$                      | J                                                            | $E_k = \frac{1}{2}mv^2$                     |
| Lagrange function                      | $L$                        | J                                                            | $L(q, \dot{q}) = T(q, \dot{q}) - V(q)$      |
| Linear strain, relative elongation     | $\epsilon, e$              |                                                              | $\epsilon = \Delta l/l$                     |
| Mass                                   | $m$                        | kg                                                           |                                             |
| Modulus of elasticity, Young's modulus | $E$                        | Pa                                                           | $E = \sigma/\epsilon$                       |
| Moment of inertia                      | $I, J$                     | $\text{kg} \cdot \text{m}^2$                                 | $I = \sum m_i r_i^2$                        |
| Momentum                               | $\mathbf{p}$               | $\text{kg} \cdot \text{m} \cdot \text{s}^{-1}$               | $\mathbf{p} = m\mathbf{v}$                  |
| Normal stress                          | $\sigma$                   | Pa                                                           | $\sigma = F/A$                              |
| Potential energy                       | $E_p$                      | J                                                            | $E_p = \int -\mathbf{F} \cdot d\mathbf{s}$  |
| Power                                  | $P$                        | W                                                            | $P = dW/dt$                                 |
| Pressure                               | $p, P$                     | Pa, $\text{N} \cdot \text{m}^{-2}$                           | $p = F/A$                                   |
| Reduced mass                           | $\mu$                      | kg                                                           | $\mu = m_1m_2/(m_1 + m_2)$                  |
| Relative density                       | $d$                        |                                                              | $d = \rho/\rho^0$                           |
| Shear modulus                          | $G$                        | Pa                                                           | $G = \tau/\gamma$                           |
| Shear strain                           | $\gamma$                   |                                                              | $\gamma = \Delta x/d$                       |
| Shear stress                           | $\tau$                     | Pa                                                           | $\tau = F/A$                                |
| Sound energy flux                      | $P, P_a$                   | W                                                            | $P = dE/dt$                                 |
| Specific volume                        | $v$                        | $\text{m}^3 \cdot \text{kg}^{-1}$                            | $v = V/\mu = 1/\rho$                        |
| Surface density                        | $\rho_A, \rho_S$           | $\text{kg} \cdot \text{m}^{-2}$                              | $\rho_A = m/A$                              |
| Surface tension                        | $\gamma, \sigma$           | $\text{N} \cdot \text{m}^{-1}, \text{J} \cdot \text{m}^{-2}$ | $\gamma = dW/dA$                            |
| Torque, moment of a force              | $\mathbf{T}, (\mathbf{M})$ | $\text{N} \cdot \text{m}$                                    | $\mathbf{T} = \mathbf{r} \times \mathbf{F}$ |
| Viscosity (dynamic)                    | $\eta, \mu$                | $\text{Pa} \cdot \text{s}$                                   | $\tau_{xz} = \lambda(dv_x/dz)$              |
| Volume (or bulk) strain                | $\theta$                   |                                                              | $\theta = \Delta V/V_0$                     |
| Weight                                 | $G, (W, P)$                | N                                                            | $G = m \cdot g$                             |
| Work                                   | $W, w$                     | J                                                            | $W = \int \mathbf{F} \cdot d\mathbf{s}$     |

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| J. Solid state                          |                            |                                                      |                                                                          |
|-----------------------------------------|----------------------------|------------------------------------------------------|--------------------------------------------------------------------------|
| Name                                    | Symbol                     | SI unit                                              | Definition                                                               |
| Acceptor ionization energy              | $E_a$                      | J                                                    |                                                                          |
| Bragg angle                             | $\theta$                   | rad                                                  | $n\lambda = 2d \sin \theta$                                              |
| Bloch function                          | $u_k(\mathbf{r})$          | $\text{m}^{-3/2}$                                    | $\psi(\mathbf{r}) = u_k(\mathbf{r}) \exp(ik \cdot \mathbf{r})$           |
| Burgers vector                          | $\mathbf{b}$               | m                                                    |                                                                          |
| Charge density of electrons             | $\rho$                     | $\text{C} \cdot \text{m}^{-3}$                       | $\rho(\mathbf{r}) = -e\psi^*(\mathbf{r})\psi(\mathbf{r})$                |
| Circular wave vector:                   |                            |                                                      |                                                                          |
| For particles ( $\mathbf{k}$ )          | $\mathbf{k}, \mathbf{q}$   | $\text{m}^{-1}$                                      | $\mathbf{k} = 2\pi/\lambda$                                              |
| For phonons ( $\mathbf{q}$ )            |                            |                                                      |                                                                          |
| Conductivity tensor                     | $\sigma_{ik}$              | $\text{S} \cdot \text{m}^{-1}$                       | $\sigma = \rho^{-1}$                                                     |
| Curie temperature                       | $T_C$                      | K                                                    |                                                                          |
| Debye circular frequency                | $\omega_D$                 | $\text{s}^{-1}$                                      |                                                                          |
| Debye circular wavenumber               | $q_D$                      | $\text{m}^{-1}$                                      |                                                                          |
| Debye-Waller factor                     | $B, D$                     |                                                      |                                                                          |
| Density of states                       | $N_E$                      | $\text{J}^{-1} \cdot \text{m}^{-3}$                  | $N_E = dN(E)/dE$                                                         |
| Density of vibrational modes (spectral) | $N_\omega, g$              | $\text{s} \cdot \text{m}^{-3}$                       | $N_\omega = dN(\omega)/d\omega$                                          |
| Diffusion coefficient                   | $D$                        | $\text{m}^2 \cdot \text{s}^{-1}$                     | $dN/dt = -DA \, dn/dx$                                                   |
| Diffusion length                        | $L$                        | m                                                    | $L = (D\tau)^{1/2}$                                                      |
| Displacement vector of an ion           | $\mathbf{u}$               | m                                                    | $\mathbf{u} = \mathbf{R} - \mathbf{R}_0$                                 |
| Donor ionization energy                 | $E_d$                      | J                                                    |                                                                          |
| Effective mass                          | $m^*$                      | kg                                                   |                                                                          |
| Equilibrium position vector of an ion   | $\mathbf{R}_0$             | m                                                    |                                                                          |
| Fermi energy                            | $E_F$                      | J                                                    |                                                                          |
| Gap energy                              | $E_g$                      |                                                      |                                                                          |
| Grüneisen parameter                     | $\gamma, \Gamma$           |                                                      | $\gamma = \alpha V/\kappa C_V$                                           |
| Hall coefficient                        | $A_H, R_H$                 | $\text{m}^3 \cdot \text{C}^{-1}$                     | $\mathbf{E} = \rho \cdot \mathbf{j} + R_H(\mathbf{B} \times \mathbf{j})$ |
| Lattice plane spacing                   | $d$                        | m                                                    |                                                                          |
| Lattice vector                          | $\mathbf{R}, \mathbf{R}_0$ | m                                                    |                                                                          |
| Lorenz coefficient                      | $L$                        | $\text{V}^2 \cdot \text{K}^{-2}$                     | $L = \lambda/\sigma T$                                                   |
| Madelung constant                       | $\alpha$                   |                                                      | $E_{\text{coul}} = \frac{\alpha N_A Z_+ Z_- e^2}{4\pi\epsilon_0 R_0}$    |
| Mobility                                | $\mu$                      | $\text{m}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$ | $\mu = v_{\text{drift}}/E$                                               |
| Mobility ratio                          | $b$                        |                                                      | $b = \mu_n/\mu_p$                                                        |
| Neel temperature                        | $T_N$                      | K                                                    |                                                                          |
| Number density, number concentration    | $n$                        | $\text{m}^{-3}$                                      |                                                                          |
| Order parameters:                       |                            |                                                      |                                                                          |
| Long range                              | $s$                        |                                                      |                                                                          |
| Short range                             | $\sigma$                   |                                                      |                                                                          |
| Order of reflection                     | $n$                        |                                                      |                                                                          |
| Particle position vector:               |                            |                                                      |                                                                          |
| Electron                                | $\mathbf{r}$               | m                                                    |                                                                          |
| Ion position                            | $\mathbf{R}_j$             | m                                                    |                                                                          |
| Peltier coefficient                     | $\Pi$                      | V                                                    |                                                                          |
| Reciprocal lattice vector (circular)    | $\mathbf{G}$               | $\text{m}^{-1}$                                      | $\mathbf{G} \cdot \mathbf{R} = 2\pi m$                                   |



TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| J. Solid state (continued)                                |                                                                                                                  |                                                    |                                                                                    |
|-----------------------------------------------------------|------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|------------------------------------------------------------------------------------|
| Name                                                      | Symbol                                                                                                           | SI unit                                            | Definition                                                                         |
| Relaxation time                                           | $\tau$                                                                                                           | s                                                  | $\tau = 1/v_F$                                                                     |
| Residual resistivity                                      | $\rho_R$                                                                                                         | m                                                  |                                                                                    |
| Resistivity tensor                                        | $\boldsymbol{\rho}$                                                                                              | $\Omega \cdot \text{m}$                            | $\boldsymbol{E} = \boldsymbol{\rho} \cdot \boldsymbol{j}$                          |
| Temperature                                               | $\theta$                                                                                                         | K                                                  |                                                                                    |
| Thermal conductivity tensor                               | $\boldsymbol{\lambda}$                                                                                           | $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ | $\boldsymbol{J}_q = -\boldsymbol{\lambda} \cdot \text{grad } T$                    |
| Thermoelectric force                                      | $E$                                                                                                              | V                                                  |                                                                                    |
| Thomson coefficient                                       | $\mu$                                                                                                            | $\text{V} \cdot \text{K}^{-1}$                     |                                                                                    |
| Translation vectors for the reciprocal lattice (circular) | $\boldsymbol{b}_1; \boldsymbol{b}_2; \boldsymbol{b}_3$<br>$\boldsymbol{a}^*; \boldsymbol{b}^*; \boldsymbol{c}^*$ | $\text{m}^{-1}$                                    | $\boldsymbol{a}_i \cdot \boldsymbol{b}_k = 2\pi\delta_{ik}$                        |
| Translation vectors for crystal lattice                   | $\boldsymbol{a}_1; \boldsymbol{a}_2; \boldsymbol{a}_3$<br>$\boldsymbol{a}; \boldsymbol{b}; \boldsymbol{c}$       | m                                                  | $\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$ |
| Work function                                             | $\Phi$                                                                                                           | J                                                  | $\Phi = E_\infty - E_F$                                                            |
| K. Space and time                                         |                                                                                                                  |                                                    |                                                                                    |
| Name                                                      | Symbol                                                                                                           | SI unit                                            | Definition                                                                         |
| Acceleration                                              | $\boldsymbol{a}, (g)$                                                                                            | $\text{m} \cdot \text{s}^{-2}$                     | $\boldsymbol{a} = d\boldsymbol{v}/dt$                                              |
| Angular velocity                                          | $\omega$                                                                                                         | $\text{rad} \cdot \text{s}^{-1}, \text{s}^{-1}$    | $\omega = d\phi/dt$                                                                |
| Area                                                      | $A, A_s, S$                                                                                                      | $\text{m}^2$                                       |                                                                                    |
| Breadth                                                   | $b$                                                                                                              | m                                                  |                                                                                    |
| Cartesian space coordinates                               | $x, y, z$                                                                                                        | m                                                  |                                                                                    |
| Circular frequency, angular frequency                     | $\omega$                                                                                                         | $\text{rad} \cdot \text{s}^{-1}, \text{s}^{-1}$    | $\omega = 2\pi\nu$                                                                 |
| Diameter                                                  | $d$                                                                                                              | m                                                  |                                                                                    |
| Distance                                                  | $d$                                                                                                              | m                                                  |                                                                                    |
| Frequency                                                 | $\nu, f$                                                                                                         | Hz                                                 | $\nu = 1/T$                                                                        |
| Generalized coordinate                                    | $q, q_i$                                                                                                         | (varies)                                           |                                                                                    |
| Height                                                    | $h$                                                                                                              | m                                                  |                                                                                    |
| Length                                                    | $l$                                                                                                              | m                                                  |                                                                                    |
| Length of arc                                             | $s$                                                                                                              | m                                                  |                                                                                    |
| Path length                                               | $s$                                                                                                              | m                                                  |                                                                                    |
| Period                                                    | $T$                                                                                                              | s                                                  | $T = t/N$                                                                          |
| Plane angle                                               | $\alpha, \beta, \gamma,$<br>$\theta, \phi$                                                                       | rad, $l$                                           | $\alpha = s/r$                                                                     |
| Position vector                                           | $\boldsymbol{r}$                                                                                                 | m                                                  | $\boldsymbol{r} = x\boldsymbol{i} + y\boldsymbol{j} + z\boldsymbol{k}$             |
| Radius                                                    | $r$                                                                                                              | m                                                  |                                                                                    |
| Relaxation time, time constant                            | $\tau, T$                                                                                                        | s                                                  | $\tau =  dt/d \ln x $                                                              |
| Solid angle                                               | $\omega, \Omega$                                                                                                 | sr, l                                              | $\Omega = A/r^2$                                                                   |
| Speed                                                     | $v, u, w, c$                                                                                                     | $\text{m} \cdot \text{s}^{-1}$                     | $v =  \boldsymbol{v} $                                                             |
| Spherical polar coordinates                               | $r, \theta, \phi$                                                                                                | m, l, l                                            |                                                                                    |
| Thickness                                                 | $d, \delta$                                                                                                      | m                                                  |                                                                                    |
| Time                                                      | $t$                                                                                                              | s                                                  |                                                                                    |
| Velocity                                                  | $\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{w}, \boldsymbol{c}$                                                 | $\text{m} \cdot \text{s}$                          | $\boldsymbol{v} = d\boldsymbol{r}/dt$                                              |
| Volume                                                    | $V, (v)$                                                                                                         | $\text{m}^3$                                       |                                                                                    |

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| L. Spectroscopy                                                       |                                                   |                                 |                                                                                   |
|-----------------------------------------------------------------------|---------------------------------------------------|---------------------------------|-----------------------------------------------------------------------------------|
| Name                                                                  | Symbol                                            | SI unit                         | Definition                                                                        |
| Asymmetry parameter                                                   | $\kappa$                                          |                                 | $\kappa = \frac{2B - A - C}{A - C}$                                               |
| Centrifugal distortion constants:                                     |                                                   |                                 |                                                                                   |
| A reduction                                                           | $\Delta_J \Delta_{JK} \Delta_K \delta_J \delta_K$ | $\text{m}^{-1}$                 |                                                                                   |
| S reduction                                                           | $D_J D_{JK} D_K d_1 d_2$                          |                                 |                                                                                   |
| Degeneracy, statistical weight                                        | $g, d, \beta$                                     |                                 |                                                                                   |
| Electric dipole moment of a molecule                                  | $\mathbf{p}, \boldsymbol{\mu}$                    | $\text{C} \cdot \text{m}$       | $E_{\text{p}} = -\mathbf{p} \cdot \mathbf{E}$                                     |
| Electron spin resonance (ESR), electron paramagnetic resonance (EPR): |                                                   |                                 |                                                                                   |
| Hyperfine coupling constant:                                          |                                                   |                                 |                                                                                   |
| In liquids                                                            | $a, A$                                            | Hz                              | $\hat{H}_{\text{ms}}/h = a\hat{\mathbf{S}} \cdot \mathbf{I}$                      |
| In solids                                                             | $T$                                               | Hz                              | $\hat{H}_{\text{ms}}/h = \hat{\mathbf{S}} \cdot \mathbf{T} \cdot \mathbf{I}$      |
| g factor                                                              | $g$                                               |                                 | $h\nu = g\mu_{\text{B}}B$                                                         |
| Electronic term                                                       | $T_{\text{e}}$                                    | $\text{m}^{-1}$                 | $T_{\text{e}} = E_{\text{e}}/hc$                                                  |
| Harmonic vibration wave-number                                        | $\omega_{\text{e}}, \omega_{\text{r}}$            | $\text{m}^{-1}$                 |                                                                                   |
| Inertial defect                                                       | $\Delta$                                          | $\text{kg} \cdot \text{m}^2$    | $\Delta = I_{\text{C}} - I_{\text{A}} - I_{\text{B}}$                             |
| Interatomic distances:                                                |                                                   |                                 |                                                                                   |
| Equilibrium distance                                                  | $r_{\text{e}}$                                    | m                               |                                                                                   |
| Ground state distance                                                 | $r_0$                                             | m                               |                                                                                   |
| Substitution structure distance                                       | $r_{\text{s}}$                                    | m                               |                                                                                   |
| Zero-point average distance                                           | $r_{\text{z}}$                                    | m                               |                                                                                   |
| Longitudinal relaxation time                                          | $T_1$                                             | s                               |                                                                                   |
| Nuclear magnetic resonance (NMR), chemical shift, $\delta$ scale      | $\delta$                                          |                                 | $\delta = 10^6(\nu - \nu_0)/\nu_0$                                                |
| Coupling constant, direct (dipolar)                                   | $D_{\text{AB}}$                                   | Hz                              |                                                                                   |
| Magnetogyric ratio                                                    | $\gamma$                                          | $\text{C} \cdot \text{kg}^{-1}$ | $\gamma = 2\pi\mu/Ih$                                                             |
| Shielding constant                                                    | $\sigma_{\text{A}}$                               |                                 | $B_{\text{A}} = (1 - \sigma_{\text{A}})B$                                         |
| Spin-spin coupling constant                                           | $J_{\text{AB}}$                                   | Hz                              | $H/h = J_{\text{AB}}\mathbf{I}_{\text{A}} \cdot \mathbf{I}_{\text{B}}$            |
| Principal moments of inertia                                          | $I_{\text{A}}, I_{\text{B}}, I_{\text{C}}$        | $\text{kg} \cdot \text{m}^2$    | $I_{\text{A}} \leq I_{\text{B}} \leq I_{\text{C}}$                                |
| Rotational constants:                                                 |                                                   |                                 |                                                                                   |
| In frequency                                                          | $A; B; C$                                         | Hz                              | $A = h/8\pi^2I_{\text{A}}$                                                        |
| In wavenumber                                                         | $\tilde{A}; \tilde{B}; \tilde{C}$                 | $\text{m}^{-1}$                 | $\tilde{A} = h/8\pi^2I_{\text{A}}$                                                |
| Rotational term                                                       | $F$                                               | $\text{m}^{-1}$                 | $F = E_{\text{rot}}/hc$                                                           |
| Spin orbit coupling constant                                          | $A$                                               | $\text{m}^{-1}$                 | $T_{\text{s.o.}} = A \langle \tilde{\mathbf{L}} \cdot \tilde{\mathbf{S}} \rangle$ |
| Total term                                                            | $T$                                               | $\text{m}^{-1}$                 | $T = E_{\text{tot}}/hc$                                                           |
| Transition dipole moment of a molecule                                | $\mathbf{M}, \mathbf{R}$                          | $\text{C} \cdot \text{m}$       | $M = \int \psi' \mathbf{p} \psi'' d\tau$                                          |

**TABLE 2.2** Physical and Chemical Symbols and Definitions (*Continued*)

| L. Spectroscopy ( <i>continued</i> )  |                                                 |                                |                                                                                     |                             |
|---------------------------------------|-------------------------------------------------|--------------------------------|-------------------------------------------------------------------------------------|-----------------------------|
| Name                                  | Symbol                                          | SI unit                        | Definition                                                                          |                             |
| Transition frequency                  | $\nu$                                           | Hz                             | $\nu = (E' - E'')/h$                                                                |                             |
| Transition wavenumber                 | $\tilde{\nu}, (\nu)$                            | $\text{m}^{-1}$                | $\tilde{\nu} = T' - T''$                                                            |                             |
| Transverse relaxation time            | $T_2$                                           | s                              |                                                                                     |                             |
| Vibrational anharmonicity constant    | $\omega_e X_e; \chi_{rs}; g_w$                  | $\text{m}^{-1}$                |                                                                                     |                             |
| Vibrational coordinates:              |                                                 |                                |                                                                                     |                             |
| Internal coordinates                  | $R_i, r_i, \theta_j$ , etc.                     |                                |                                                                                     |                             |
| Normal coordinates, dimensionless     | $q_r$                                           |                                |                                                                                     |                             |
| Mass adjusted                         | $Q_r$                                           |                                |                                                                                     |                             |
| Vibrational force constants:          |                                                 |                                |                                                                                     |                             |
| Diatomic                              | $f, (k)$                                        | $\text{J} \cdot \text{m}^{-2}$ | $f = \partial^2 V/\partial r^2$                                                     |                             |
| Polyatomic                            |                                                 |                                |                                                                                     |                             |
| Dimensionless normal coordinates      | $\phi_{\text{rst} \dots}, k_{\text{rst} \dots}$ | $\text{m}^{-1}$                |                                                                                     |                             |
| Internal coordinates                  | $f_{ij}$                                        | (varies)                       | $f_{ij} = \partial^2 V/\partial r_i \partial r_j$                                   |                             |
| Symmetry coordinates                  | $F_{ij}$                                        | (varies)                       | $F_{ij} = \partial^2 V/\partial S_i \partial S_j$                                   |                             |
| Vibrational quantum numbers           | $\nu_r; l_t$                                    |                                |                                                                                     |                             |
| Vibrational term                      | $G$                                             | $\text{m}^{-1}$                | $G = E_{\text{vib}}/hc$                                                             |                             |
|                                       |                                                 |                                |                                                                                     |                             |
| Angular momentum types                |                                                 | Operator symbol                | Quantum number symbol                                                               |                             |
|                                       |                                                 |                                | Total                                                                               | Z axis      z axis          |
| Electron orbital                      | $\hat{L}$                                       | $L$                            | $M_L$                                                                               | $\Lambda$                   |
| One electron only                     | $\hat{l}$                                       | $l$                            | $m_l$                                                                               | $\lambda$                   |
| Electron orbital + spin               | $\hat{L} + \hat{S}$                             |                                |                                                                                     | $\Omega = \Lambda + \Sigma$ |
| Electron spin                         | $\hat{S}$                                       | $S$                            | $M_S$                                                                               | $\sigma$                    |
| One electron only                     | $\hat{s}$                                       | $s$                            | $m_s$                                                                               | $\Sigma$                    |
| Internal vibrational:                 |                                                 |                                |                                                                                     |                             |
| Spherical top                         | $\hat{I}$                                       | $I(l\xi)$                      |                                                                                     | $K_I$                       |
| Other                                 | $\hat{J}, \hat{\pi}$                            |                                |                                                                                     | $l(l\xi)$                   |
| Nuclear orbital (rotational)          | $\hat{R}$                                       | $R$                            |                                                                                     | $K_R, k_R$                  |
| Nuclear spin                          | $\hat{I}$                                       | $I$                            | $M_I$                                                                               |                             |
| Sum of $J + I$                        | $\hat{F}$                                       | $F$                            | $M_F$                                                                               |                             |
| Sum of $N + S$                        | $\hat{J}$                                       | $J$                            | $M_J$                                                                               | $K, k$                      |
| Sum of $R + L(+j)$                    | $\hat{N}$                                       | $N$                            |                                                                                     | $K, k$                      |
| M. Thermodynamics                     |                                                 |                                |                                                                                     |                             |
| Name                                  | Symbol                                          | SI unit                        | Definition                                                                          |                             |
| Absolute activity                     | $\lambda$                                       |                                | $\lambda_{\text{B}} = \exp(\mu_{\text{B}}/RT)$                                      |                             |
| Activity (referenced to Henry's law): |                                                 |                                |                                                                                     |                             |
| Concentration basis                   | $a_{\text{c}}$                                  |                                | $a_{\text{c,B}} = \exp \left[ \frac{\mu_{\text{B}} - \mu_{\text{B}}^*}{RT} \right]$ |                             |

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| M. Thermodynamics (continued)                     |                            |                                               |                                                              |
|---------------------------------------------------|----------------------------|-----------------------------------------------|--------------------------------------------------------------|
| Name                                              | Symbol                     | SI unit                                       | Definition                                                   |
| Molality basis                                    | $a_m$                      |                                               | $a_{m,B} = \exp \left[ \frac{\mu_B - \mu_B^*}{RT} \right]$   |
| Mole fraction basis                               | $a_x$                      |                                               | $a_{x,B} = \exp \left[ \frac{\mu_B - \mu_B^*}{RT} \right]$   |
| Activity (referenced to Raoult's law)             | $a$                        |                                               | $a_B = \exp \left[ \frac{\mu_B - \mu_B^*}{RT} \right]$       |
| Activity coefficient (referenced to Henry's law): |                            |                                               |                                                              |
| Concentration basis                               | $\gamma_c$                 |                                               | $a_{c,B} = \gamma_{c,B} c_B / c^0$                           |
| Molality basis                                    | $\gamma_m$                 |                                               | $a_{m,B} = \gamma_{m,B} m_B / m^0$                           |
| Mole fraction basis                               | $\gamma_x$                 |                                               | $a_{x,B} = \gamma_{x,B} x_B$                                 |
| Activity coefficient (referenced to Raoult's law) | $f$                        |                                               | $f_B = a_B / x_B$                                            |
| Affinity of reaction                              | $A$                        | $\text{J} \cdot \text{mol}^{-1}$              | $A = -(\partial G / \partial \xi)_{p,T}$                     |
| Celsius temperature                               | $\theta, t$                | $^{\circ}\text{C}$                            | $\theta / ^{\circ}\text{C} = T / \text{K} - 273.15$          |
| Chemical potential                                | $\mu$                      | $\text{J} \cdot \text{mol}^{-1}$              | $\mu_B = (\partial G / \partial n_B)_{T,p,n}$                |
| Compressibility:                                  |                            |                                               |                                                              |
| Isentropic                                        | $\kappa_S$                 | $\text{Pa}^{-1}$                              | $\kappa_S = -(1/V)(\partial V / \partial p)_S$               |
| Isothermal                                        | $\kappa_T$                 | $\text{Pa}^{-1}$                              | $\kappa_T = -(1/V)(\partial V / \partial p)_T$               |
| Compressibility factor                            | $Z$                        |                                               | $Z = pV_m / RT$                                              |
| Cubic expansion coefficient                       | $\alpha, \alpha_v, \gamma$ | $\text{K}^{-1}$                               | $\alpha = (1/V)(\partial V / \partial T)_p$                  |
| Enthalpy                                          | $H$                        | $\text{J}$                                    | $H = U + pV$                                                 |
| Entropy                                           | $S$                        | $\text{J} \cdot \text{K}^{-1}$                | $dS \geq dq/T$                                               |
| Equilibrium constant                              | $K^0, K$                   |                                               | $K^{\circ} = \exp(-\Delta_r G^{\circ} / RT)$                 |
| Equilibrium constant:                             |                            |                                               |                                                              |
| Concentration basis                               | $K_c$                      | $(\text{mol} \cdot \text{m}^{-3})^{\sum \nu}$ | $K_c = \Pi c^{\nu}$                                          |
| Molality basis                                    | $K_m$                      | $(\text{mol} \cdot \text{m}^{-1})^{\sum \nu}$ | $K_m = \Pi m^{\nu}$                                          |
| Pressure basis                                    | $K_p$                      | $\text{Pa}^{\sum \nu}$                        | $K_p = \Pi p^{\nu}$                                          |
| Fugacity                                          | $f$                        | $\text{Pa}$                                   | $f_B = \lambda_B \lim_{p \rightarrow 0} (p_B / \lambda_B)_T$ |
| Fugacity coefficient                              | $\phi$                     |                                               | $\phi_B = f_B / p_B$                                         |
| Gibbs energy                                      | $G$                        | $\text{J}$                                    | $G = H - TS$                                                 |
| Heat                                              | $q, Q$                     | $\text{J}$                                    |                                                              |
| Heat capacity:                                    |                            |                                               |                                                              |
| At constant pressure                              | $C_p$                      | $\text{J} \cdot \text{K}^{-1}$                | $C_p = (\partial H / \partial T)_p$                          |
| At constant volume                                | $C_v$                      | $\text{J} \cdot \text{K}^{-1}$                | $C_v = (\partial U / \partial T)_v$                          |
| Helmholtz energy                                  | $A$                        | $\text{J}$                                    | $A = U - TS$                                                 |
| Internal energy                                   | $U$                        |                                               | $\Delta U = q + w$                                           |
| Ionic strength:                                   |                            |                                               |                                                              |
| Concentration basis                               | $I_c, I$                   | $\text{mol} \cdot \text{kg}^{-3}$             | $I_c = \frac{1}{2} \sum m_B z_B^2$                           |
| Molality basis                                    | $I_m, I$                   | $\text{mol} \cdot \text{kg}^{-1}$             | $I_m = \frac{1}{2} \sum m_B z_B^2$                           |
| Joule-Thomson coefficient                         | $\mu, \mu_{JT}$            | $\text{K} \cdot \text{Pa}^{-1}$               | $\mu = (\partial T / \partial p)_H$                          |
| Linear expansion coefficient                      | $\alpha_1$                 | $\text{K}^{-1}$                               | $\alpha_1 = (1/l)(\partial l / \partial T)$                  |
| Massieu function                                  | $J$                        | $\text{J} \cdot \text{K}^{-1}$                | $J = -A/T$                                                   |
| Molar quantity $X$                                | $X_m$                      | (varies)                                      | $X_m = X/n$                                                  |
| Osmotic coefficient:                              |                            |                                               |                                                              |
| Molality basis                                    | $\phi_m$                   |                                               | $\phi_m = (\mu_A^* - \mu_A) / (RT m_A \sum m_B)$             |
| Mole fraction basis                               | $\phi_x$                   |                                               | $\phi_x = (\mu_A - \mu_A^*) / (RT \ln x_A)$                  |

**TABLE 2.2** Physical and Chemical Symbols and Definitions (*Continued*)

| M. Thermodynamics ( <i>continued</i> )   |                  |                                       |                                               |
|------------------------------------------|------------------|---------------------------------------|-----------------------------------------------|
| Name                                     | Symbol           | SI unit                               | Definition                                    |
| Osmotic pressure (ideal dilute solution) | $\Pi$            | Pa                                    | $\Pi = c_B RT$                                |
| Partial molar quantity $X$               | $X_B$            | (varies)                              | $X = (\partial X / \partial n_B)_{T,p,n}$     |
| Planck function                          | $Y$              | $J \cdot K^{-1}$                      | $Y = -G/T$                                    |
| Pressure coefficient                     | $\beta$          | $Pa \cdot K^{-1}$                     | $\beta = (\partial P / \partial T)_V$         |
| Ratio of heat capacities                 | $\gamma$         |                                       | $\gamma = C_p / C_v$                          |
| Relative pressure coefficient            | $\alpha_p$       | $K^{-1}$                              | $\alpha_p = (1/p)(\partial p / \partial T)_V$ |
| Second virial coefficient                | $B$              | $m^3 \cdot mol^{-1}$                  | $pV_m = RT(1 + B/V_m + \cdots)$               |
| Specific quantity $X$                    | $x$              | (varies)                              | $x = X/m$                                     |
| Standard chemical potential              | $\mu^0$          | $J \cdot mol^{-1}$                    |                                               |
| Standard partial molar enthalpy          | $H^0$            | $J \cdot mol^{-1}$                    | $H^0 = \mu^0 + TS$                            |
| Standard partial molar entropy           | $S^0$            | $J \cdot mol^{-1} \cdot K^{-1}$       | $S^0 = -(\partial \mu^0 / \partial T)$        |
| Standard reaction enthalpy               | $\Delta_r H^0$   | $J \cdot mol^{-1}$                    | $\Delta_r H^0 = \sum \nu H^0$                 |
| Standard reaction entropy                | $\Delta_r S^0$   | $J \cdot mol^{-1} \cdot K^{-1}$       | $\Delta_r S^0 = \sum \nu S^0$                 |
| Standard reaction Gibbs energy           | $\Delta_r G^0$   | $J \cdot mol^{-1}$                    | $\Delta_r G^0 = \sum \nu \mu^0$               |
| Surface tension                          | $\gamma, \sigma$ | $J \cdot m^{-2},$<br>$N \cdot m^{-1}$ | $\gamma = (\partial G / \partial A_s)_{T,p}$  |
| Thermodynamic temperature                | $T$              | K                                     |                                               |
| Work                                     | $w, W$           | J                                     |                                               |

Symbols used as subscripts to denote a chemical reaction or process:

|     |                                   |     |                               |
|-----|-----------------------------------|-----|-------------------------------|
| ads | adsorption                        | mix | mixing of fluids              |
| at  | atomization                       | r   | reaction in general           |
| c   | combustion reaction               | sol | solution of solute in solvent |
| dil | dilution of a solution            | sub | sublimation (solid to gas)    |
| f   | formation reaction                | trs | transition (two phases)       |
| fus | melting, fusion (solid to liquid) |     |                               |

Recommended superscripts:

|    |                                     |          |                   |
|----|-------------------------------------|----------|-------------------|
| +  | activated complex, transition state | $\infty$ | infinite solution |
| E  | excess quantity                     | *        | pure substance    |
| id | ideal                               | °        | standard          |

N. Transport properties

| Name                         | Symbol       | SI unit                       | Definition                |
|------------------------------|--------------|-------------------------------|---------------------------|
| Coefficient of heat transfer | $h, (k, K)$  | $W \cdot m^{-2} \cdot K^{-1}$ | $h = J_q / \Delta T$      |
| Diffusion coefficient        | $D$          | $m^2 \cdot s^{-1}$            | $D = J_n / (dc/dl)$       |
| Flux (of a quantity $X$ )    | $J_X, J$     | (varies)                      | $J_X = A^{-1} dX/dt$      |
| Heat flow rate               | $\phi$       | W                             | $\phi = dq/dt$            |
| Heat flux                    | $J_q$        | $W \cdot m^{-2}$              | $J_q = \phi/A$            |
| Mass flow rate               | $q_m, m$     | $kg \cdot s^{-1}$             | $q_m = dm/dt$             |
| Mass transfer coefficient    | $k_d$        | $m \cdot s^{-1}$              |                           |
| Thermal conductance          | $G$          | $W \cdot K^{-1}$              | $G = \phi / \Delta T$     |
| Thermal conductivity         | $\lambda, k$ | $W \cdot m^{-1} \cdot K^{-1}$ | $\lambda = J_q / (dT/dl)$ |

TABLE 2.2 Physical and Chemical Symbols and Definitions (Continued)

| N. Transport properties (continued)                          |            |                                  |                                                                    |
|--------------------------------------------------------------|------------|----------------------------------|--------------------------------------------------------------------|
| Name                                                         | Symbol     | SI unit                          | Definition                                                         |
| Thermal diffusivity                                          | $a$        | $\text{m}^2 \cdot \text{s}^{-1}$ | $a = \lambda/\rho c_p$                                             |
| Thermal resistance                                           | $R$        | $\text{K} \cdot \text{W}^{-1}$   | $R = 1/G$                                                          |
| Volume flow rate                                             | $q_v, V$   | $\text{m}^3 \cdot \text{s}^{-1}$ | $q_v = dV/dt$                                                      |
| Dimensionless quantities:                                    |            |                                  |                                                                    |
| Alfvén number                                                | $Al$       |                                  | $Al = v(\rho\mu)^{1/2}/B$                                          |
| Cowling number                                               | $Co$       |                                  | $Co = B^2/\mu\rho v^2$                                             |
| Euler number                                                 | $Eu$       |                                  | $Eu = \Delta p/\rho v^2$                                           |
| Fourier number                                               | $Fo$       |                                  | $Fo = at/l^2$                                                      |
| Fourier number for mass transfer in binary mixtures          | $Fo^*$     |                                  | $Fo^* = Dt/l^2$                                                    |
| Froude number                                                | $Fr$       |                                  | $Fr = v/(lg)^{1/2}$                                                |
| Grashof number                                               | $Gr$       |                                  | $Gr = l^3 go \Delta T \rho^2/\eta^2$                               |
| Grashof number for mass transfer in binary mixtures          | $Gr^*$     |                                  | $Gr^* = l^3 g (\partial\rho/\partial x)_{T,p} (\Delta x \pi/\eta)$ |
| Hartmann number                                              | $Ha$       |                                  | $Ha = Bl(\kappa/\eta)^{1/2}$                                       |
| Knudsen number                                               | $Kn$       |                                  | $Kn = \lambda/l$                                                   |
| Lewis number                                                 | $Le$       |                                  | $Le = a/D$                                                         |
| Mach number                                                  | $Ma$       |                                  | $Ma = v/c$                                                         |
| Magnetic Reynolds number                                     | $Rm, Re_m$ |                                  | $Rm = \nu\mu\kappa l$                                              |
| Nusselt number                                               | $Nu$       |                                  | $Nu = hl/k$                                                        |
| Nusselt number for mass transfer in binary mixtures          | $Nu^*$     |                                  | $Nu^* = k_d l/D$                                                   |
| Péclet number                                                | $Pe$       |                                  | $Pe = \nu l/a$                                                     |
| Péclet number for mass transfer in binary mixtures           | $Pe^*$     |                                  | $Pe^* = \nu l/D$                                                   |
| Prandtl number                                               | $Pr$       |                                  | $Pr = \eta/\rho a$                                                 |
| Rayleigh number                                              | $Ra$       |                                  | $Ra = l^3 g \alpha \Delta T \rho/\eta a$                           |
| Reynolds number                                              | $Re$       |                                  | $Re = \rho \nu l/\eta$                                             |
| Schmidt number                                               | $Sc$       |                                  | $Sc = \eta/\rho D$                                                 |
| Sherwood number                                              | $Sh$       |                                  | $Sh = k_d l/D$                                                     |
| Stanton number                                               | $St$       |                                  | $St = h/\rho v c_p$                                                |
| Stanton number for mass transfer in binary mixtures          | $St^*$     |                                  | $St^* = k_d/v$                                                     |
| Strouhal number                                              | $Sr$       |                                  | $Sr = lf/v$                                                        |
| Weber number                                                 | $We$       |                                  | $We = \rho v^2 l/\gamma$                                           |
| Symbols used in the definitions of dimensionless quantities: |            |                                  |                                                                    |
| Acceleration of free fall                                    | $g$        | Pressure                         | $p$                                                                |
| Area                                                         | $A$        | Speed                            | $v$                                                                |
| Cubic expansion coefficient                                  | $\alpha$   | Speed of sound                   | $c$                                                                |
| Density                                                      | $\rho$     | Surface tension                  | $\gamma$                                                           |
| Frequency                                                    | $f$        | Temperature                      | $T$                                                                |
| Length                                                       | $l$        | Time                             | $t$                                                                |
| Mass                                                         | $m$        | Viscosity                        | $\eta$                                                             |
| Mean free path                                               | $\lambda$  | Volume                           | $V$                                                                |
| Mole fraction                                                | $x$        |                                  |                                                                    |

**TABLE 2.3** Mathematical Symbols and Abbreviations

| Symbol or abbreviation          | Meaning                                                 |
|---------------------------------|---------------------------------------------------------|
| +                               | Plus                                                    |
| −                               | Minus                                                   |
| ±                               | Plus or minus                                           |
| ∓                               | Minus or plus                                           |
| ≡                               | Identically equal to                                    |
| $\times$ , center dot           | Multiplied by ( $ab$ , $a \times b$ , $a \cdot b$ )     |
| ÷                               | Divided by ( $a/b$ , $ab^{-1}$ )                        |
| ≠                               | Not equal to                                            |
| ≈                               | Approximately equal to                                  |
| ≍                               | Asymptotically equal to                                 |
| >                               | Greater than                                            |
| <                               | Less than                                               |
| ≫                               | Much greater than                                       |
| ≪                               | Much less than                                          |
| ≥                               | Greater than or equal to                                |
| ≤                               | Less than or equal to                                   |
| $\propto$ , ~                   | Proportional to                                         |
| →                               | Tends to, approaches                                    |
| ∞                               | Infinity                                                |
| $a$                             | Magnitude of $a$                                        |
| $a^n$                           | $n$ th power of $a$                                     |
| $\sqrt[n]{a}$ , $a^{1/n}$       | $n$ th root of $a$                                      |
| $\sqrt{a}$ , $a^{1/2}$          | Square root of $a$                                      |
| $\langle a \rangle$ , $\bar{a}$ | Mean value of $a$                                       |
| $\prod_{i=1}^n a_i$ , $\Pi a_i$ | Product of $a_i$                                        |
| $\log a$ or $\log_{10} a$       | Common (or Briggsian) logarithm to the base 10 of $a$   |
| $\log_a b$                      | Logarithm to the base $a$ of $b$                        |
| $\ln b$ , $\log_e b$            | Natural (Napierian) logarithm (to the base $e$ ) of $b$ |
| $e$                             | Base (2.718) of natural system of logarithms            |
| $\pi$                           | Pi (3.1416)                                             |
| $i$                             | Imaginary quantity, square root of minus one            |
| $n!$                            | $n$ factorial ( $n! = 1 \cdot 2 \cdot 3 \cdots n$ )     |
| ∠                               | Angle                                                   |
| ⊥                               | Perpendicular to                                        |
|                                 | Parallel to                                             |
| $a^\circ$                       | $a$ degrees (angle)                                     |
| $a'$                            | $a$ minutes (angle); $a$ prime                          |
| $a''$                           | $a$ seconds (angle); $a$ double prime                   |
| $\sin a$                        | sine of $a$                                             |
| $\cos a$                        | cosine of $a$                                           |
| $\tan a$                        | tangent of $a$                                          |
| $\cot a$                        | cotangent of $a$                                        |
| $\sec a$                        | secant of $a$                                           |
| $\csc a$                        | cosecant of $a$                                         |
| $\arcsin a$ , $\sin^{-1} a$     | Inverse sine of $a$ (angle whose sine is $a$ )          |
| $\arccos a$ , $\cos^{-1} a$     | Inverse cosine of $a$ (angle whose cosine is $a$ )      |
| $\arctan a$ , $\tan^{-1} a$     | Inverse tangent of $a$ (angle whose tangent is $a$ )    |
| $\sinh a$                       | Hyperbolic sine of $a$                                  |
| $\cosh a$                       | Hyperbolic cosine of $a$                                |
| $\tanh a$                       | Hyperbolic tangent of $a$                               |

**TABLE 2.3** Mathematical Symbols and Abbreviations (*Continued*)

| Symbol or abbreviation                       | Meaning                                                      |
|----------------------------------------------|--------------------------------------------------------------|
| $\coth a$                                    | Hyperbolic cotangent of $a$                                  |
| $P(x, y)$                                    | Rectangular coordinate of point $P$                          |
| $P(r, \theta)$                               | Polar coordinate of point $P$                                |
| $f(x), F(x)$                                 | Function of $x$                                              |
| $\Delta x$                                   | Increment of $x$                                             |
| $dy$                                         | Total differential of $y$                                    |
| $\frac{dy}{dx}$ or $f'(x)$                   | Derivative of $y = f(x)$ with respect to $x$                 |
| $\frac{d^2y}{dx^2}$ or $f''(x)$              | Second derivative of $y = f(x)$ with respect to $x$          |
| $\frac{\partial z}{\partial x}$              | Partial derivative of $z$ with respect to $x$                |
| $\frac{\partial^2 z}{\partial x \partial y}$ | Second partial derivative of $z$ with respect to $x$ and $y$ |
| $\int$                                       | Integral of                                                  |
| $\int_a^b$                                   | Integral between the limits $a$ and $b$                      |
| $\lim_{x \rightarrow a} f(x)$                | limit of $f(x)$ as $x$ tends to $a$                          |
| $\sum_{i=1}^n$                               | Summation of $a_i$ between the limits 1 and $n$              |

**TABLE 2.4** SI Prefixes

| Submultiple | Prefix | Symbol | Multiple  | Prefix | Symbol |
|-------------|--------|--------|-----------|--------|--------|
| $10^{-1}$   | deci   | d      | 10        | deka   | da     |
| $10^{-2}$   | centi  | c      | $10^2$    | hecto  | h      |
| $10^{-3}$   | milli  | m      | $10^3$    | kilo   | k      |
| $10^{-6}$   | micro  | $\mu$  | $10^6$    | mega   | M      |
| $10^{-9}$   | nano   | n      | $10^9$    | giga   | G      |
| $10^{-12}$  | pico   | p      | $10^{12}$ | tera   | T      |
| $10^{-15}$  | femto  | f      | $10^{15}$ | peta   | P      |
| $10^{-18}$  | atto   | a      | $10^{18}$ | exa    | E      |
| $10^{-21}$  | zepto  | z      | $10^{21}$ | zetta  | Z      |
| $10^{-24}$  | yocto  | y      | $10^{24}$ | yotta  | Y      |



TABLE 2.4 SI Prefixes (Continued)

| Numerical (multiplying) prefixes |                   |        |                |        |                 |
|----------------------------------|-------------------|--------|----------------|--------|-----------------|
| Number                           | Prefix            | Number | Prefix         | Number | Prefix          |
| 0.5                              | hemi              | 19     | nonadeca       | 39     | nonatriaconta   |
| 1                                | mono              | 20     | icosa          | 40     | tetraconta      |
| 1.5                              | sesqui            | 21     | henicosa       | 41     | hentetraconta   |
| 2                                | di (bis)*         | 22     | docosa         | 42     | dotetraconta    |
| 3                                | tri (tris)*       | 23     | tricoso        | 43     | tritetraconta   |
| 4                                | tetra (tetrakis)* | 24     | tetracoso      | 44     | tetratetraconta |
| 5                                | penta             | 25     | pentacoso      | 45     | pentatetraconta |
| 6                                | hexa              | 26     | hexacoso       | 46     | hexatetraconta  |
| 7                                | hepta             | 27     | heptacoso      | 47     | heptatetraconta |
| 8                                | octa              | 28     | octacoso       | 48     | octatetraconta  |
| 9                                | nona              | 29     | nonacoso       | 49     | nonatetraconta  |
| 10                               | deca              | 30     | triaconta      | 50     | pentaconta      |
| 11                               | undeca            | 31     | hentriaconta   | 60     | hexaconta       |
| 12                               | dodeca            | 32     | dotriaconta    | 70     | heptaconta      |
| 13                               | trideca           | 33     | tritriaconta   | 80     | octaconta       |
| 14                               | tetradeca         | 34     | tetratriaconta | 90     | nonaconta       |
| 15                               | pentadeca         | 35     | pentatriaconta | 100    | hecta           |
| 16                               | hexadeca          | 36     | hexatriaconta  | 110    | decahecta       |
| 17                               | heptadeca         | 37     | heptatriaconta | 120    | icosahecta      |
| 18                               | octadeca          | 38     | octatriaconta  | 130    | triacontahecta  |

\* In the case of complex entities such as organic ligands (particularly if they are substituted) the multiplying prefixes bis-, tris-, tetrakis-, pentakis-, . . . are used, i.e., -kis is added starting from tetra-. The modified entity is often placed within parentheses to avoid ambiguity.

TABLE 2.5 Greek Alphabet

| Capital   | Lower case | Name    | Capital  | Lower case | Name    |
|-----------|------------|---------|----------|------------|---------|
| A         | $\alpha$   | Alpha   | N        | $\nu$      | Nu      |
| B         | $\beta$    | Beta    | $\Xi$    | $\xi$      | Xi      |
| $\Gamma$  | $\gamma$   | Gamma   | O        | $o$        | Omicron |
| $\Delta$  | $\delta$   | Delta   | $\Pi$    | $\pi$      | Pi      |
| E         | $\epsilon$ | Epsilon | P        | $\rho$     | Rho     |
| Z         | $\zeta$    | Zeta    | $\Sigma$ | $\sigma$   | Sigma   |
| H         | $\eta$     | Eta     | T        | $\tau$     | Tau     |
| $\Theta$  | $\theta$   | Theta   | Y        | $\upsilon$ | Upsilon |
| I         | $\iota$    | Iota    | $\Phi$   | $\phi$     | Phi     |
| K         | $\kappa$   | Kappa   | X        | $\chi$     | Chi     |
| $\Lambda$ | $\lambda$  | Lambda  | $\Psi$   | $\psi$     | Psi     |
| M         | $\mu$      | Mu      | $\Omega$ | $\omega$   | Omega   |

TABLE 2.6 Abbreviations and Standard Letter Symbols

|                                                   |                    |                                       |                            |
|---------------------------------------------------|--------------------|---------------------------------------|----------------------------|
| Abampere                                          | abamp              | Angular momentum                      | $\pi$                      |
| Absolute                                          | abs                | Angular momentum terms                | $j, J, l, L, N$            |
| Absolute activity                                 | $\lambda$          | Angular velocity                      | $\omega$                   |
| Absorbance (decaidic)                             | $A$                | Anhydrous                             | anhyd                      |
| Absorbance (napierian)                            | $B$                | Approximate (circa)                   | ca.                        |
| Absorptance                                       | $\alpha$           | Aqueous solution                      | aq                         |
| Absorption coefficient, linear decaidic           | $a, K$             | Aqueous solution at infinite dilution | aq, $\infty$               |
| Absorption coefficient, linear napierian          | $\alpha$           | Are, unit of area                     | a                          |
| Absorption coefficient, molar decaidic            | $\mu, \epsilon$    | Area                                  | $A, S$                     |
| Absorption coefficient, molar napierian           | $\kappa$           | Area per molecule                     | $a, \sigma$                |
| Absorption index                                  | $k$                | Astronomical unit                     | AU                         |
| Acceleration                                      | $a$                | Asymmetry parameter                   | $\kappa$                   |
| Acceleration due to gravity                       | $g, g_n$           | Atmosphere, unit of pressure          | atm                        |
| Acetyl                                            | Ac                 | Atomic mass                           | $m_a$                      |
| Acoustic absorption factor                        | $\alpha_a$         | Atomic mass constant                  | $m_u$                      |
| Acoustic dissipation factor                       | $\delta$           | Atomic mass unit                      | amu                        |
| Acoustic reflection factor                        | $\rho$             | Atomic number                         | $Z$                        |
| Acoustic transmission factor                      | $\tau$             | Atomic percent                        | at. %                      |
| Activation energy                                 | $E_a$              | Atomic weight                         | at. wt.                    |
| Activity (referenced to Raoult's law)             | $a$                | Average                               | av                         |
| Activity (referenced to Henry's law):             |                    | Average linear gas velocity           | $\mu$                      |
| Concentration basis                               | $a_c$              | Avogadro constant                     | $L, N_A$                   |
| Molality basis                                    | $a_m$              | Axial angular momentum                | $\lambda, \Lambda, \Omega$ |
| Mole fraction basis                               | $a_x$              | Axial spin angular momentum           | $\sigma, \Sigma$           |
| Activity (radioactive)                            | $A$                | Bandwidth (10%) of a spectral filter  | $\Delta\lambda_{0.1}$      |
| Activity coefficient (referenced to Raoult's law) | $f$                | Band variance                         | $\sigma^2$                 |
| Activity coefficient (referenced to Henry's law): |                    | Bar, unit of pressure                 | bar                        |
| Concentration basis                               | $\gamma_c$         | Barn, unit of area                    | b                          |
| Molality basis                                    | $\gamma_m$         | Barrel                                | bbl                        |
| Mole fraction basis                               | $\gamma_x$         | Base of natural logarithms            | $e$                        |
| Adjusted retention time                           | $t'_R$             | Becquerel                             | Bq                         |
| Adjusted retention volume                         | $V'_R$             | Bed volume                            | $V_g$                      |
| Admittance                                        | $Y$                | Beta particle                         | $\beta$                    |
| Affinity of reaction                              | $A$                | Bloch function                        | $u_k(\mathbf{r})$          |
| Alcohol                                           | alc                | Body-centered cubic                   | bcc                        |
| Alfvén number                                     | $Al$               | Bohr                                  | $b$                        |
| Alkaline                                          | alk                | Bohr magneton                         | $\mu_B$                    |
| Alpha particle                                    | $\alpha$           | Bohr radius                           | $a_0$                      |
| Alternating current                               | ac                 | Boiling point                         | bp                         |
| Amorphous                                         | am                 | Boltzmann constant                    | $k, k_B$                   |
| Amount concentration                              | $c$                | Bragg angle                           | $\theta$                   |
| Amount of substance                               | $n$                | Breadth                               | $b$                        |
| Ampere                                            | $A$                | British thermal unit                  | Btu                        |
| Amplification factor                              | $\mu$              | Bulk modulus                          | $K$                        |
| Angle of optical rotation                         | $\alpha$           | Bulk strain                           | $\theta$                   |
| Angstrom                                          | $\text{\AA}, A$    | Burgers vector                        | $\mathbf{b}$               |
| Angular dispersion                                | $d\theta/d\lambda$ | Butyl                                 | Bu                         |
|                                                   |                    | Calorie, unit of energy               | cal                        |
|                                                   |                    | Calorie, international steam table    | cal <sub>IT</sub>          |
|                                                   |                    | Candela                               | cd                         |
|                                                   |                    | Capacitance                           | $C$                        |

**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                           |                  |                                             |                            |
|-------------------------------------------|------------------|---------------------------------------------|----------------------------|
| Capacity, volume                          | $Q_V$            | Concentration of solute in stationary phase | $C_S$                      |
| Capacity, weight                          | $Q_W$            | Condensed phase (solid or liquid)           | cd                         |
| Cartesian space coordinates               | $x, y, z$        | Conductance                                 | $G$                        |
| Celsius temperature                       | $t, \theta$      | Conductivity                                | $\gamma, \kappa$           |
| Centimeter-gram-second system             | cgs              | Conductivity cell constant                  | $K_{\text{cell}}$          |
| Centrifugal distortion constants:         |                  | Conductivity tensor                         | $\sigma_{ik}$              |
| A reduction                               | $\Delta, \delta$ | Contact angle                               | $\theta$                   |
| S reduction                               | $D, d$           | Coordinate, position vector                 | $r$                        |
| Charge density of electrons               | $\rho$           | Coulomb                                     | C                          |
| Charge number of electrochemical reaction | $n$              | Counts per minute                           | cpm, c/m                   |
| Charge number of an ion                   | $z$              | Coupling constant, direct dipolar           | $D_{AB}$                   |
| Chemically pure                           | CP               | Critical density                            | $d_c$                      |
| Chemical potential                        | $\mu$            | Critical temperature                        | $t_c$                      |
| Chemical shift                            | $\delta$         | Cross section                               | $\sigma$                   |
| Circa (approximate)                       | ca.              | Crystalline                                 | cr, cryst                  |
| Circular frequency                        | $\omega$         | Cubic                                       | cub                        |
| Circular wave vector:                     |                  | Cubic expansion coefficient                 | $\alpha, \alpha_v, \gamma$ |
| For particles                             | $k$              | Curie                                       | Ci                         |
| For phonons                               | $q$              | Cycles per second                           | Hz                         |
| Circumference divided by the diameter     | $\pi$            | Curie temperature                           | $T_c$                      |
| Citrate                                   | Cit              | Dalton (atomic mass unit)                   | Da                         |
| Coefficient of heat transfer              | $h$              | Day                                         | d                          |
| Collision cross section                   | $\sigma$         | Debye, unit of electric dipole              | D                          |
| Collision diameter                        | $d$              | Debye circular frequency                    | $\omega_D$                 |
| Collision frequency                       | $Z$              | Debye circular wave-number                  | $q_D$                      |
| Collision frequency factor                | $z$              | Debye-Waller factor                         | $D, B$                     |
| Collision number                          | $Z$              | Decay constant (radioactive)                | $\lambda$                  |
| Column volume                             | $V_{\text{col}}$ | Decibel                                     | dB                         |
| Compare (confer)                          | cf.              | Decompose                                   | dec                        |
| Complex refractive index                  | $\hat{n}$        | Degeneracy, statistical weight              | $d, g, \beta$              |
| Component of angular momentum             | $k, K, m, M$     | Degree of dissociation                      | $\alpha$                   |
| Compressibility:                          |                  | Degrees Baume                               | $^{\circ}\text{Be}$        |
| Isentropic                                | $\kappa_S$       | Degrees Celsius                             | $^{\circ}\text{C}$         |
| Isothermal                                | $\kappa_T$       | Degrees Fahrenheit                          | $^{\circ}\text{F}$         |
| Compression factor                        | $Z$              | Density (mass)                              | $\rho, \gamma$             |
| Compression modulus                       | $K$              | Density, critical                           | $d_c$                      |
| Compton wavelength of electron            | $\lambda_c$      | Density, relative                           | $d$                        |
| Compton wavelength of neutron             | $\lambda_{c,n}$  | Density of liquid phase                     | $\rho_L$                   |
| Compton wavelength of proton              | $\lambda_{c,p}$  | Density of states                           | $N_E, \rho$                |
| Concentration (amount of substance)       | $c$              | Density of vibrational modes (spectral)     | $N_{\omega}$               |
| Concentration (mass)                      | $\gamma$         | Detect, determine (d)                       | det(d)                     |
| Concentration at peak maximum             | $C_{\text{max}}$ | Determination                               | detn                       |
| Concentration of solute in mobile phase   | $C_M$            | Deuteron                                    | d                          |
|                                           |                  | Diamagnetic shielding factor                | $1 + \sigma$               |
|                                           |                  | Diameter                                    | $d$                        |
|                                           |                  | Dielectric polarization                     | $P$                        |
|                                           |                  | Differential thermal analysis               | DTA                        |
|                                           |                  | Diffusion coefficient                       | $D$                        |
|                                           |                  | Diffusion coefficient, liquid film          | $D_f$                      |

**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                                    |                 |                                                       |            |
|----------------------------------------------------|-----------------|-------------------------------------------------------|------------|
| Diffusion coefficient, mobile phase                | $D_M$           | Electron magnetic moment                              | $\mu_e$    |
| Diffusion coefficient, stationary phase            | $D_S$           | Electron paramagnetic resonance                       | EPR        |
| Diffusion current                                  | $i_d$           | Electron radius                                       | $r_e$      |
| Diffusion length                                   | $L$             | Electron rest mass                                    | $m_e$      |
| Diffusion rate constant, mass transfer coefficient | $k_d$           | Electron spin resonance                               | ESR        |
| Dilute                                             | dil             | Electronvolt                                          | eV         |
| Dirac delta function                               | $\delta$        | Electrostatic unit                                    | esu        |
| Direct current                                     | dc              | Elementary charge                                     | $e$        |
| Direct dipolar coupling constant                   | $D_{AB}$        | Elution volume, exclusion chromatography              | $V_e$      |
| Disintegration energy                              | $Q$             | Emittance                                             | $\epsilon$ |
| Disintegrations per minute                         | dpm             | By blackbody                                          | $M_{bb}$   |
| Displacement vector of an ion                      | $u$             | Energy                                                | $E$        |
| Dissociation energy                                | $D, E_d$        | Energy density                                        | $w, \rho$  |
| From ground state                                  | $D_0$           | Energy per electron hole pair of ion pair in detector | $\epsilon$ |
| From the potential minimum                         | $D_e$           | Enthalpy                                              | $H$        |
| Distribution ratio                                 | $D$             | Entropy                                               | $S$        |
| Donor ionization energy                            | $E_d$           | Entropy unit                                          | e.u.       |
| Dropping mercury electrode                         | dme             | Equilibrium constant                                  | $K, K^0$   |
| Dyne, unit of force                                | dyn             | Concentration basis                                   | $K_c$      |
| Einstein transition probabilities                  | $A, B$          | Molality basis                                        | $K_m$      |
| Spontaneous emission                               | $A_{nm}$        | Pressure basis                                        | $K_p$      |
| Stimulated absorption                              | $B_{mn}$        | Equilibrium position vector of an ion                 | $R_0$      |
| Stimulated emission                                | $B_{nm}$        | Equivalent weight                                     | equiv wt   |
| Electric charge                                    | $Q$             | Erg, unit of energy                                   | erg        |
| Electric current                                   | $I$             | Especially                                            | esp.       |
| Electric current density                           | $j, J$          | et alii (and others)                                  | et al.     |
| Electric dipole moment of a molecule               | $p, \mu$        | et cetera (and so forth)                              | etc.       |
| Electric displacement                              | $D$             | Ethyl                                                 | Et         |
| Electric field gradient                            | $q$             | Ethylenediamine                                       | en         |
| Electric field strength                            | $E$             | Ethylenediamine- $N, N, N', N'$ -tetraacetic acid     | EDTA       |
| Electric flux                                      | $\Psi$          | Euler number                                          | $Eu$       |
| Electric mobility                                  | $u, \mu$        | Exempli gratia (for example)                          | e.g.       |
| Electric polarizability of a molecule              | $\alpha$        | Expansion coefficient                                 | $\alpha$   |
| Electric potential                                 | $V, \phi$       | Exponential                                           | exp        |
| Electric potential difference                      | $U, \Delta V$   | Extent of reaction                                    | $\xi$      |
| Electric susceptibility                            | $\chi_e$        | Fano factor                                           | $F$        |
| Electrical conductivity                            | $\sigma$        | Farad                                                 | $F$        |
| Electrical conductance                             | $G$             | Faraday constant                                      | $F$        |
| Electrical resistance                              | $R$             | Fermi, unit of length                                 | $f$        |
| Electrochemical transfer coefficient               | $\alpha$        | Fermi energy                                          | $E_F$      |
| Electrokinetic potential                           | $\zeta$         | Film tension                                          | $\Sigma_f$ |
| Electromagnetic unit                               | emu             | Film thickness                                        | $h, t$     |
| Electromotive force                                | $E, \text{emf}$ | Fine structure constant                               | $\alpha$   |
| Electron                                           | $e^-, e$        | Finite change                                         | $\Delta$   |
| Electron affinity                                  | $E_{ea}$        | First radiation constant                              | $c_1$      |
|                                                    |                 | Flow rate                                             | $q$        |
|                                                    |                 | Flow rate, column chromatography                      | $F_c$      |
|                                                    |                 | Fluid phase (gas or liquid)                           | fl         |
|                                                    |                 | Fluidity                                              | $\phi$     |

**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                     |                  |                                                |                    |
|-------------------------------------|------------------|------------------------------------------------|--------------------|
| Fluorescent efficiency              | $\Phi_F$         | Helmholtz energy                               | $A$                |
| Fluorescent power                   | $P_F$            | Henry                                          | H                  |
| Flux                                | $F, J$           | Hertz                                          | Hz                 |
| Focal length                        | $f$              | Hexagonal                                      | hex                |
| Foot                                | ft               | Horsepower                                     | hp                 |
| For example (exempli gratia)        | e.g.             | Hour                                           | h                  |
| Force                               | $F$              | Hygroscopic                                    | hygr               |
| Force constant (vibrational levels) | $k$              | Hyperfine coupling constant                    | $a, A$             |
| Formal concentration                | $F$              | Hyperfine coupling tensor                      | $T$                |
| Fourier number                      | $Fo$             | ibidem (in the same place)                     | ibid.              |
| Franklin, unit of electric charge   | Fr               | id est (that is)                               | i.e.               |
| Freezing point                      | fp               | Ignition                                       | ign                |
| Frequency                           | $f, \nu$         | Impedance                                      | $Z$                |
| Friction coefficient                | $f, \mu$         | Inch                                           | in                 |
| Froude number                       | $Fr$             | Indices of a family of crystallographic planes | $hkl$              |
| Fugacity                            | $f$              | Indirect spin-spin coupling constant           | $J_{AB}$           |
| Fugacity coefficient                | $\phi$           | Inductance                                     | $L$                |
| Gallon                              | gal              | Inertial defect                                | $\Delta$           |
| Galvani potential difference        | $\Delta\phi$     | Infinitesimal change                           | $\delta$           |
| Gamma, unit of mass                 | $\gamma$         | Infrared                                       | ir                 |
| Gamma radiation                     | $\gamma$         | Inner column volume                            | $V_i$              |
| Gap energy (solid state)            | $E_g$            | Inner electric potential                       | $\phi$             |
| Gas (physical state)                | $g$              | Inner electrode potential                      | $\phi$             |
| Gas constant                        | $R$              | Inorganic                                      | inorg              |
| Gauss                               | G                | Inside diameter                                | i.d.               |
| $g$ factor                          | $g$              | Insoluble                                      | insol              |
| Gibbs energy                        | $G$              | Interatomic distances:                         |                    |
| Grade                               | grad             | Equilibrium distance                           | $r_e$              |
| Grain, unit of mass                 | gr               | Ground-state distance                          | $r_0$              |
| Gram                                | g                | Substitution structure distance                | $r_s$              |
| Grand partition function            | $\Xi$            | Zero-point average distance                    | $r_z$              |
| Grashof number                      | $Gr$             | Internal energy                                | $U$                |
| Gravimetric                         | grav             | Interstitial (outer) volume                    | $V_o$              |
| Gravitational constant              | $G$              | In the place cited (loco citato)               | loc. cit.          |
| Gray                                | Gy               | In the same place                              | ibid.              |
| Grüneisen parameter                 | $\gamma, \Gamma$ | In the work cited                              | op. cit.           |
| Half-life                           | $t_{1/2}$        | Ionic conductivity                             | $\lambda, \Lambda$ |
| Half-wave potential                 | $E_{1/2}$        | Ionic strength                                 | $I$                |
| Hall coefficient                    | $A_H, R_H$       | Concentration basis                            | $I_c$              |
| Hamilton function                   | $H$              | Molality basis                                 | $I_m$              |
| Harmonic vibration wave-number      | $\omega$         | Ionization energy                              | $E_i$              |
| Hartmann number                     | $Ha$             | Irradiance                                     | $E$                |
| Hartree energy                      | $E_h$            | Joule                                          | J                  |
| Heat                                | $q, Q$           | Joule-Thomson coefficient                      | $\mu, \mu_{JT}$    |
| Heat capacity                       | $C$              | Kelvin                                         | K                  |
| At constant pressure                | $C_p$            | Kilocalorie                                    | kcal               |
| At constant volume                  | $C_v$            | Kilogram                                       | kg                 |
| Heat flow rate                      | $\phi$           | Kilogram-force                                 | kgf                |
| Heat flux                           | $J$              | Kilowatt-hour                                  | kWh                |
| Hectare, unit of area               | ha               | Kinematic viscosity                            | $\nu, \phi$        |
| Height                              | $h$              |                                                |                    |
| Helion                              | h                |                                                |                    |

**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                      |                                      |                                          |                    |
|--------------------------------------|--------------------------------------|------------------------------------------|--------------------|
| Kinetic energy                       | $K, T, E_k$                          | Mass number                              | $A$                |
| Knudsen number                       | $Kn$                                 | Mass of atom                             | $m, m_a$           |
| Kovats retention indices             | RI                                   | Mass transfer coefficient                | $k_d$              |
| Lagrange function                    | $L$                                  | Matrix volume                            | $V_g$              |
| Lambda, unit of volume               | $\lambda$                            | Maximum                                  | max                |
| Landé $g$ -factor                    | $g, g_e$                             | Maxwell, unit of magnetic flux           | Mx                 |
| Larmor circular frequency            | $\omega_L$                           | Mean ionic activity                      | $a_{\pm}$          |
| Larmor frequency                     | $\nu_L$                              | Mean ionic activity coefficient          | $\gamma_{\pm}$     |
| Lattice plane spacing                | $d$                                  | Mean ionic mobility                      | $W_{\pm}$          |
| Lattice vector                       | $\mathbf{R}, \mathbf{R}_0$           | Melting point                            | mp                 |
| Lattice vectors                      | $\mathbf{a}, \mathbf{b}, \mathbf{c}$ | Metallic                                 | met                |
| Length                               | $l, L$                               | Metastable                               | $m$                |
| Length of arc                        | $s$                                  | Metastable peaks                         | $m^*$              |
| Lewis number                         | $Le$                                 | Meter                                    | m                  |
| Light year                           | l.y.                                 | Methyl                                   | Me                 |
| Limit (mathematics)                  | lim                                  | Micrometer                               | $\mu\text{m}$      |
| Linear expansion coefficient         | $\alpha_1$                           | Micron                                   | $\mu$              |
| Linear reciprocal dispersion         | $D^{-1}, d\lambda/dx$                | Mile                                     | mi                 |
| Linear strain                        | $e, \epsilon$                        | Miller indices                           | $h, l, k$          |
| Liquid                               | l, lq                                | Milliequivalent                          | meq                |
| Liquid crystal                       | lc                                   | Millimeters of mercury, unit of pressure | mmHg               |
| Liter                                | L, l                                 | Millimole                                | mM                 |
| loco citato (in the place cited)     | loc. cit.                            | Minimum                                  | min                |
| Logarithm, common                    | log                                  | Minute                                   | m, min             |
| Logarithm, base $e$                  | ln                                   | Mixture                                  | mixt               |
| Longitudinal relaxation time         | $T_1$                                | Mobility                                 | $\mu$              |
| Lorenz coefficient                   | $L$                                  | Mobility ratio                           | $b$                |
| Loss angle                           | $\delta$                             | Modulus of elasticity                    | $E$                |
| Lumen                                | lm                                   | Molal                                    | $m$                |
| Luminous intensity                   | $I$                                  | Molality                                 | $b$                |
| Lux                                  | lx                                   | Molar                                    | $M, \mathbf{M}$    |
| Mach number                          | $Ma$                                 | Molar (decadic) absorption coefficient   | $\epsilon$         |
| Madelung constant                    | $\alpha$                             | Molar ionic conductivity                 | $\lambda, \Lambda$ |
| Magnetic dipole moment of a molecule | $\mathbf{m}, \boldsymbol{\mu}$       | Molar magnetic susceptibility            | $\chi_m$           |
| Magnetic field strength              | $\mathbf{H}$                         | Molar mass                               | $M$                |
| Magnetic flux                        | $\Phi$                               | Molar quantity $X$                       | $X_m$              |
| Magnetic flux density                | $B$                                  | Molar refraction                         | $R, R_m$           |
| Magnetic moment of protons in water  | $\mu_p/\mu_B$                        | Molar volume                             | $V_m$              |
| Magnetic quantum number              | $M_j$                                | Mole                                     | mol                |
| Magnetic Reynolds number             | $Rm$                                 | Mole fraction, condensed phase           | $x$                |
| Magnetic susceptibility              | $\kappa, \chi$                       | Gaseous mixtures                         | $y$                |
| Magnetic vector potential            | $\mathbf{A}$                         | Mole percent                             | mol %              |
| Magnetizability                      | $\xi$                                | Molecular weight                         | mol wt             |
| Magnetization                        | $\mathbf{M}$                         | Moment of inertia                        | $I, J$             |
| Magnetogyric ratio                   | $\gamma$                             | Momentum                                 | $p$                |
| Mass                                 | $m$                                  | Monoclinic                               | mn                 |
| Mass absorption coefficient          | $\mu/\rho, \mu_m$                    | Monomeric form                           | mon                |
| Mass concentration                   | $\gamma, \rho$                       | Muon, negative                           | $\mu^-$            |
| Mass density                         | $\rho$                               | Muon, positive                           | $\mu^+$            |
| Mass flow rate                       | $q_m$                                |                                          |                    |
| Mass fraction                        | $w$                                  |                                          |                    |
| Massieu function                     | $J$                                  |                                          |                    |

**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                                 |                                                |                           |                                       |
|-------------------------------------------------|------------------------------------------------|---------------------------|---------------------------------------|
| Mutual inductance                               | $M, L$                                         | Outer diameter            | o.d.                                  |
| Napierian absorbance                            | $B$                                            | Outer electric potential  | $\psi$                                |
| Napierian base                                  | $e$                                            | Overall order of reaction | $n$                                   |
| Napierian molar absorption coefficient          | $\kappa$                                       | Overpotential             | $\eta$                                |
| Neel temperature                                | $T_N$                                          | Oxalate                   | Ox                                    |
| Net retention volume                            | $V_N$                                          | Oxidant                   | ox                                    |
| Neutrino                                        | $\nu_e$                                        | Packing uniformity factor | $\lambda$                             |
| Neutron                                         | $n$                                            | Page(s)                   | p. (pp.)                              |
| Neutron magnetic moment                         | $\mu_N$                                        | Parsec, unit of length    | pc                                    |
| Neutron number                                  | $N$                                            | Partial molar quantity    | $X$                                   |
| Neutron rest mass                               | $m_n$                                          | Partial order of reaction | $n_B$                                 |
| Newton                                          | $N$                                            | Particle diameter         | $d_p$                                 |
| Normal concentration                            | $N$                                            | Particle position vector: |                                       |
| Normal stress                                   | $\sigma$                                       | Electron                  | $\mathbf{r}$                          |
| Nuclear magnetic resonance                      | NMR                                            | Ion position              | $\mathbf{R}_j$                        |
| Nuclear magneton                                | $\mu_N$                                        | Partition coefficient     | $K$                                   |
| Nuclear spin angular momentum                   | $I$                                            | Partition function        | $q, Q, z, Z, \Omega$                  |
| Nucleon number                                  | $A$                                            | Partition ratio           | $k'$                                  |
| Number concentration                            | $C$                                            | Parts per billion, volume | ng/mL                                 |
| Number density                                  | $n$                                            | Parts per billion, weight | ng/g                                  |
| Number of entities                              | $N$                                            | Parts per million, volume | $\mu\text{g/mL}$                      |
| Numerical aperture                              | NA                                             | Parts per million, weight | $\mu\text{g/g}$                       |
| Nusselt number                                  | $Nu$                                           | Pascal                    | Pa                                    |
| Obstruction factor                              | $\gamma$                                       | Path length (absorbing)   | $l$                                   |
| Oersted, unit of magnetic field                 | Oe                                             | Peak asymmetry factor     | $AF$                                  |
| Ohm                                             | $\Omega$                                       | Peak resolution           | $Rs$                                  |
| opere citato (in the work cited)                | op. cit.                                       | Péclet number             | $Pe$                                  |
| Optical speed                                   | $f/\text{number}$                              | Peltier coefficient       | $\Pi$                                 |
| Orbital angular momentum:                       |                                                | Percent                   | %                                     |
| Quantum number                                  | $L = 0, 1, 2, 3, \dots$                        | Period of time            | $T$                                   |
| Series symbol                                   | $S, P, D, F, \dots$                            | Permeability              | $\mu$                                 |
| Orbital angular momentum (molecules):           |                                                | Permeability of vacuum    | $\mu_0$                               |
| Quantum number                                  | $\Lambda = 0, 1, 2, \dots$                     | Permittivity              | $\epsilon$                            |
| Symbol                                          | $\Sigma, \Pi, \Delta, \dots$                   | Permittivity of vacuum    | $\epsilon_0$                          |
| Orbital angular momenta of individual electrons | $l = 0, 1, 2, 3, \dots$<br>$s, p, d, f, \dots$ | pH, expressed in activity | pH                                    |
| Order of Bragg reflection                       | $n$                                            | Expressed in molarity     | pH                                    |
| Order of reaction                               | $n$                                            | Phenyl                    | Ph, $\phi$                            |
| Order of reflection                             | $n$                                            | Phosphorescent efficiency | $\Phi_p$                              |
| Order parameters (solid state), long range      | $s$                                            | Phosphorescent power      | $P_p$                                 |
| Short range                                     | $\sigma$                                       | Photochemical yield       | $\phi$                                |
| Organic                                         | org                                            | Photoluminescence power   | $P$                                   |
| Orthorhombic                                    | o-rh                                           | Photon                    | $\gamma$                              |
| Osmotic coefficient                             | $\phi$                                         | Pion                      | $\pi$                                 |
| Molality basis                                  | $\phi_m$                                       | Planck constant           | $h$                                   |
| Mole fraction basis                             | $\phi_x$                                       | Planck constant/ $2\pi$   | $\hbar$                               |
| Osmotic pressure (ideal dilute solution)        | $\Pi$                                          | Planck function           | $Y$                                   |
| Ounce                                           | oz                                             | Plane angle               | $\alpha, \beta, \gamma, \theta, \phi$ |
|                                                 |                                                | Plate height              | $H$                                   |
|                                                 |                                                | Plate number, effective   | $N_{\text{eff}}$                      |
|                                                 |                                                | Poise                     | P                                     |
|                                                 |                                                | Polymeric form            | pol                                   |
|                                                 |                                                | Porosity, column          | $\epsilon$                            |
|                                                 |                                                | Positron                  | $\beta^+$                             |
|                                                 |                                                | Potential energy          | $V, \Phi, E_p$                        |
|                                                 |                                                | Pound                     | lb                                    |

TABLE 2.6 Abbreviations and Standard Letter Symbols (Continued)

|                                                                    |                                                    |                                             |                                   |
|--------------------------------------------------------------------|----------------------------------------------------|---------------------------------------------|-----------------------------------|
| Pounds per square inch                                             | psi                                                | Reciprocal lattice vector (circular)        | <b>G</b>                          |
| Powder                                                             | pwd                                                | Vectors for                                 | <b>a*, b*, c*</b>                 |
| Power                                                              | <i>p</i>                                           | Reciprocal radius of ionic atmosphere       | $\kappa$                          |
| Poynting vector                                                    | <b>S</b>                                           | Reciprocal temperature parameter, $1/kT$    | $\beta$                           |
| Prandtl number                                                     | <i>Pr</i>                                          | Reciprocal thickness of double layer        | $\kappa$                          |
| Pressure (partial)                                                 | <i>p</i>                                           | Reduced column length                       | $\lambda$                         |
| Pressure (total)                                                   | <i>p, P</i>                                        | Reduced mass                                | $\mu$                             |
| Pressure coefficient                                               | $\beta$                                            | Reduced plate height                        | <i>h</i>                          |
| Pressure, column inlet                                             | <i>p<sub>i</sub></i>                               | Reduced velocity                            | <i>v</i>                          |
| Pressure, column outlet                                            | <i>p<sub>o</sub></i>                               | Reductant                                   | red                               |
| Pressure, critical                                                 | <i>p<sub>c</sub></i>                               | Reference                                   | ref                               |
| Pressure drop                                                      | $\Delta P$                                         | Reflectance                                 | $\rho$                            |
| Pressure-gradient correction                                       | <i>j</i>                                           | Reflection plane                            | $\sigma$                          |
| Principal moments of inertia                                       | <i>I<sub>A</sub>; I<sub>B</sub>; I<sub>C</sub></i> | Refractive index                            | <i>n</i>                          |
| Principal quantum number                                           | <i>n</i>                                           | Relative permeability                       | $\mu_r$                           |
| Probability                                                        | <i>P</i>                                           | Relative permittivity (dielectric constant) | $\epsilon_r$                      |
| Probability density                                                | <i>P</i>                                           | Relative pressure coefficient               | $\alpha_p$                        |
| Product sign                                                       | $\Pi$                                              | Relative retention ratio                    | $\alpha$                          |
| Propyl                                                             | Pr                                                 | Relaxation time                             | $\tau$                            |
| Proton                                                             | <i>p</i>                                           | Rem, unit of dose equivalent                | rem                               |
| Proton magnetic resonance                                          | pmr                                                | Residual resistivity (solid state)          | $\rho_R$                          |
| Proton magnetogyric ratio                                          | $\gamma_p$                                         | Resistivity tensor                          | <b><math>\rho</math></b>          |
| Proton number                                                      | <i>Z</i>                                           | Retardation factor                          | <i>R<sub>f</sub></i>              |
| Proton rest mass                                                   | <i>m<sub>p</sub></i>                               | Retarded van der Waals constant             | <i>B, <math>\beta</math></i>      |
| Pyridine                                                           | py                                                 | Retention time                              | <i>t<sub>R</sub></i>              |
| Quadrupole interaction energy tensor                               | <b><math>\chi</math></b>                           | Retention volume                            | <i>V<sub>R</sub></i>              |
| Quadrupole moment of a molecule                                    | <i>Q, <math>\Theta</math></i>                      | Revolutions per minute                      | rpm                               |
| Quantity of electricity, electric charge                           | <i>Q</i>                                           | Reynolds number                             | <i>Re</i>                         |
| Quantum of energy                                                  | <i>h<math>\nu</math></i>                           | Rhombic                                     | rh                                |
| Quantum yield                                                      | $\phi$                                             | Rhombohedral                                | rh-hed                            |
| Rad, unit of radiation dose                                        | rad                                                | Roentgen                                    | R                                 |
| Radian                                                             | rad                                                | Root-mean-square                            | rms                               |
| Radiant energy                                                     | <i>Q, W</i>                                        | Rotational constants:                       |                                   |
| Radiant energy density                                             | $\rho, w$                                          | In frequency                                | <i>A, B, C</i>                    |
| Radiant energy flux                                                | <i>dQ/dt</i>                                       | In wavenumber                               | $\tilde{A}; \tilde{B}; \tilde{C}$ |
| Radiant exitance                                                   | <i>M</i>                                           | Rotational term (spectroscopy)              | <i>F</i>                          |
| Radiant flux received                                              | <i>E</i>                                           | Rotation-reflection                         | <i>S<sub>n</sub></i>              |
| Radiant intensity                                                  | <i>I</i>                                           | Rydberg, unit of energy                     | Ry                                |
| Radiant intensity at time <i>t</i> after termination of excitation | <i>I(t)</i>                                        | Rydberg constant                            | R, <i>R<sub>∞</sub></i>           |
| Radiant power                                                      | $\Phi$                                             | Saturated                                   | satd                              |
| Radiant power incident on sample                                   | <i>P<sub>0</sub></i>                               | Saturated calomel electrode                 | SCE                               |
| Radiofrequency                                                     | <i>rf</i>                                          | Schmidt number                              | <i>Sc</i>                         |
| Radius                                                             | <i>r</i>                                           | Second                                      | <i>s</i>                          |
| Rate of concentration change                                       | <i>r</i>                                           | Second radiation constant                   | <i>c<sub>2</sub></i>              |
| Rate constant                                                      | <i>k</i>                                           | Second virial coefficient                   | <i>B</i>                          |
| Rate of reaction                                                   | <i>v</i>                                           | Sedimentation coefficient                   | <i>s</i>                          |
| Ratio of heat capacities                                           | $\gamma$                                           | Selectivity coefficient                     | <i>k</i>                          |
| Reactance                                                          | <i>X</i>                                           |                                             |                                   |
| Reciprocal lattice                                                 | <b>a*, b*, c*</b>                                  |                                             |                                   |



**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                                                                                                 |                                       |                                                     |                     |
|-----------------------------------------------------------------------------------------------------------------|---------------------------------------|-----------------------------------------------------|---------------------|
| Self-inductance                                                                                                 | $L$                                   | Spin orbit coupling constant                        | $A$                 |
| Separation factor                                                                                               | $\alpha$                              | Spin-spin coupling constant                         | $J_{AB}$            |
| Shear modulus                                                                                                   | $G$                                   | Spin-spin (or transverse) relaxation time           | $T_2$               |
| Shear strain                                                                                                    | $\gamma$                              | Spin wavefunctions                                  | $\alpha, \beta$     |
| Shear stress                                                                                                    | $\tau$                                | Square                                              | sq                  |
| Sherwood number                                                                                                 | $Sh$                                  | Standard                                            | std                 |
| Shielding constant (NMR)                                                                                        | $\sigma$                              | Standard enthalpy of activation                     | $H^\ddagger$        |
| Short-range order parameter                                                                                     | $\sigma$                              | Standard enthalpy of formation                      | $\Delta H_f^0$      |
| Siemens                                                                                                         | $S$                                   | Standard entropy                                    | $S^0$               |
| Sievert                                                                                                         | $S_v$                                 | Standard entropy of activation                      | $\Delta S^\ddagger$ |
| Signal-to-noise ratio                                                                                           | $S/N$                                 | Standard Gibbs energy of activation                 | $\Delta G^\ddagger$ |
| Slightly                                                                                                        | sl                                    | Standard Gibbs energy of formation                  | $\Delta G_f^0$      |
| Solid                                                                                                           | c, s                                  | Standard heat capacity                              | $C_p$               |
| Solid angle                                                                                                     | $\omega, \Omega$                      | Standard hydrogen electrode                         | SHE                 |
| Solid angle over which luminescence is measured (F, fluorescence; P, phosphorescence; DF, delayed fluorescence) | $\Omega_{F(P,DF)}$                    | Standard partial molar enthalpy                     | $H^0$               |
| Solid angle over which radiation is absorbed in cell                                                            | $\Omega_A$                            | Standard partial molar entropy                      | $S^0$               |
| Solubility                                                                                                      | s                                     | Standard potential of electrochemical cell reaction | $E^0$               |
| Soluble                                                                                                         | sol                                   | Standard reaction enthalpy                          | $\Delta_r H^0$      |
| Solution                                                                                                        | soln, sln                             | Standard reaction entropy                           | $\Delta_r S^0$      |
| Solvent                                                                                                         | solv                                  | Standard reaction Gibbs energy                      | $\Delta_r G^0$      |
| Sound energy flux                                                                                               | $P, P_a$                              | Standard temperature and pressure                   | STP                 |
| Spacing between crystal diffracting planes                                                                      | $d$                                   | Stanton number                                      | $St$                |
| Species adsorbed on a substance                                                                                 | ads                                   | Statistical weight                                  | $W, \beta, \omega$  |
| Specific gravity                                                                                                | sp gr                                 | Statistical weight of atomic states                 | $g$                 |
| Specific retention volume                                                                                       | $V_g^0$                               | Stefan-Boltzmann constant                           | $\sigma$            |
| Specific surface area                                                                                           | $s$                                   | Steradian                                           | sr                  |
| Specific volume                                                                                                 | $v, v$                                | Stoichiometric number                               | $\nu$               |
| Spectral bandwidth of emission monochromator                                                                    | $\Delta\lambda_{em}$                  | Stokes                                              | St                  |
| Spectral bandwidth of excitation monochromator                                                                  | $\Delta\lambda_{ex}$                  | Summation sign                                      | $\Sigma$            |
| Spectral bandwidth of monochromator                                                                             | $\Delta\lambda_m$                     | Surface charge density                              | $\sigma$            |
| Spectral radiant energy                                                                                         | $Q_\lambda, dQ/d\lambda$              | Surface concentration                               | $\Gamma$            |
| Spectral radiant energy density:                                                                                |                                       | Surface coverage                                    | $\theta$            |
| In terms of frequency                                                                                           | $\rho_\nu, w_\nu$                     | Surface density                                     | $\rho_A, \rho_s$    |
| In terms of wavelength                                                                                          | $\rho_\nu, w_\nu$                     | Surface electric potential                          | $\chi$              |
| In terms of wavenumber                                                                                          | $\rho_{\tilde{\nu}}, w_{\tilde{\nu}}$ | Surface pressure                                    | $\pi$               |
| Spectral radiant energy flux                                                                                    | $d\phi/d\lambda$                      | Surface tension                                     | $\gamma, \sigma$    |
| Spectroscopic splitting factor                                                                                  | $g$                                   | Susceptance                                         | $B$                 |
| Speed                                                                                                           | $u, w$                                | Svedberg, unit of time                              | Sv                  |
| Speed of light:                                                                                                 |                                       | Symmetrical                                         | sym                 |
| In a medium                                                                                                     | $c$                                   | Symmetry coordinate                                 | $S$                 |
| In vacuum                                                                                                       | $c_0$                                 | Symmetry number                                     | $s, \sigma$         |
| Spherical polar coordinates                                                                                     | $r, \theta, \phi$                     | Tartrate                                            | Tart                |
| Spin angular momentum                                                                                           | $s, S$                                | Temperature                                         | $\theta, \Theta$    |
| Spin-lattice relaxation time                                                                                    | $T_1$                                 |                                                     |                     |

**TABLE 2.6** Abbreviations and Standard Letter Symbols (*Continued*)

|                                           |                              |                                              |                                                 |
|-------------------------------------------|------------------------------|----------------------------------------------|-------------------------------------------------|
| Temperature, thermodynamic                | $T$                          | Vibrational anharmonicity constant           | $\chi$                                          |
| Temperature at boiling point              | $T_b$                        | Vibrational coordinates:                     |                                                 |
| Term value spectroscopy                   | $T$                          | Internal coordinates                         | $R_i, r_i, \theta_j$ , etc.                     |
| Tesla                                     | T                            | Normal coordinates, dimensionless            | $q_i$                                           |
| Tetragonal                                | tetr                         | Mass adjusted                                | $Q_i$                                           |
| Thermal conductance                       | $G$                          | Vibrational force constants:                 |                                                 |
| Thermal conductivity                      | $\lambda, k$                 | Diatomic                                     | $f$                                             |
| Thermal diffusivity                       | $a$                          | Polyatomic, dimensionless normal coordinates | $\phi_{\text{rst}} \dots; k_{\text{rst}} \dots$ |
| Thermal resistance                        | $R$                          | Internal coordinates                         | $f_{ij}$                                        |
| Thermoelectric force                      | $E$                          | Symmetry coordinates                         | $F_{ij}$                                        |
| Thickness of diffusion layer              | $\delta$                     | Vibrational quantum number                   | $\nu$                                           |
| Thickness of layer                        | $t$                          | Vibrational term                             | $G$                                             |
| Thickness (effective) of stationary phase | $d_f$                        | Viscosity                                    | $\eta, \mu$                                     |
| Thickness of surface layer                | $\tau$                       | Vitreous substance                           | vit                                             |
| Thickness of various layers               | $\delta$                     | Volt                                         | V                                               |
| Thomson coefficient                       | $\mu, \tau$                  | Volt-ampere-reactive                         | var                                             |
| Thomson cross section                     | $\sigma_e$                   | Volta potential difference                   | $\Delta\psi$                                    |
| Time                                      | $t$                          | Volume                                       | $V, v$                                          |
| Time interval, characteristic             | $T, \tau$                    | Volume flow rate                             | $q_v$                                           |
| Tonne                                     | t, ton                       | Volume fraction                              | $\phi$                                          |
| Torr (mm of mercury)                      | Torr                         | Volume in space phase                        | $\Omega$                                        |
| Torque                                    | $T$                          | Volume liquid phase in column                | $V_L$                                           |
| Total bed volume                          | $V_{\text{tot}}$             | Volume mobile phase in column                | $V_M$                                           |
| Total term (spectroscopy)                 | $T$                          | Volume of activation                         | $\Delta^+V$                                     |
| Transconductance                          | $g_m$                        | Volume percent                               | vol %                                           |
| Transfer coefficient                      | $\alpha$                     | Volume per volume                            | v/v                                             |
| Transit time of nonretained solute        | $t_M, t_0$                   | Volume strain                                | $\theta$                                        |
| Transition                                | tr                           | Watt                                         | W                                               |
| Transition dipole moment of a molecule    | $M, R$                       | Wavefunction                                 | $\phi, \psi, \Psi$                              |
| Transition frequency                      | $\nu$                        | Wavelength                                   | $\lambda$                                       |
| Transition wavenumber                     | $\tilde{\nu}$                | Wavenumber (in a medium)                     | $\sigma$                                        |
| Translation (circular)                    | $b_1; b_2; b_3$              | Wavenumber in vacuum                         | $\tilde{\nu}$                                   |
| Translation vectors for crystal lattice   | $a_1; a_2; a_3$<br>$a; b; c$ | Weber                                        | Wb                                              |
| Transmission factor                       | $\tau$                       | Weber number                                 | $We$                                            |
| Transmittance                             | $T, \tau$                    | Weight                                       | $W$                                             |
| Transport number                          | $t$                          | Weight of liquid phase                       | $w_L$                                           |
| Transverse relaxation time                | $T_2$                        | Weight percent                               | wt %                                            |
| Triclinic                                 | tric                         | Weight per volume                            | w/v                                             |
| Trigonal                                  | trig                         | Wien displacement constant                   | $b$                                             |
| Triton (tritium nucleus)                  | t                            | Work                                         | $w, W$                                          |
| Ultrahigh frequency                       | uhf                          | Work function                                | $\Phi$                                          |
| Ultraviolet                               | uv                           | x unit                                       | $X$                                             |
| Unified atomic mass unit                  | u                            | Yard                                         | yd                                              |
| United States Pharmacopoeia               | USP                          | Young's modulus                              | $E$                                             |
| Vacuum                                    | vac                          | Zeeman splitting constant                    | $\mu_B/\hbar c$                                 |
| van der Waals constant                    | $\lambda$                    | Zone width at baseline                       | $W_b$                                           |
| Vapor pressure                            | $p, vp$                      | Zone width at one-half peak height           | $W_{1/2}$                                       |
| Velocity                                  | $u, w$                       |                                              |                                                 |
| Versus                                    | vs                           |                                              |                                                 |

**TABLE 2.7** Conversion Factors

The data were compiled by L. P. Busetth for the 13th edition; some entries have been added or modified in view of recent data and SI units.

Relations which are exact are indicated by an asterisk (\*). Factors in parentheses are also exact. Other factors are within  $\pm 5$  in the last significant figure.

| To convert                   | Into                           | Multiply by                 |
|------------------------------|--------------------------------|-----------------------------|
| Abampere                     | ampere*                        | 10                          |
| Abcoulomb                    | coulomb*                       | 10                          |
|                              | statcoulomb                    | $2.998 \times 10^{10}$      |
| Abfarad                      | farad*                         | $10^9$                      |
| Abhenry                      | henry*                         | $10^{-9}$                   |
| Abmho                        | siemens*                       | $10^9$                      |
| Abvolt                       | volt                           | $10^{-8}$                   |
| Acre                         | hectare or square hectometer   | 0.404 685 64                |
|                              | square chain (Gunter's)*       | 10                          |
|                              | square kilometer*              | 0.004 046 873               |
|                              | square meter*                  | 4046.873                    |
|                              | square mile*                   | (1/640)                     |
|                              | square rod*                    | 160                         |
|                              | square yard*                   | 4840                        |
| Acre (U.S. survey)           | square meter                   | 4046.873                    |
| Acre-foot                    | cubic foot*                    | $4.3560 \times 10^4$        |
|                              | cubic meter                    | 1233.482                    |
|                              | gallon (U.S.)                  | $3.259 \times 10^5$         |
| Acre-inch                    | cubic foot*                    | 3630                        |
|                              | cubic meter                    | 102.7902                    |
| Ampere per square centimeter | ampere per square inch*        | 6.4516                      |
| Ampere-hour                  | coulomb*                       | 3600                        |
|                              | faraday                        | 0.037 31                    |
| Ampere-turn                  | gilbert                        | 1.256 637                   |
| Ampere-turn per centimeter   | ampere-turn per inch           | 2.540                       |
| Ångström                     | meter*                         | $10^{-10}$                  |
|                              | nanometer*                     | 0.1                         |
| Apostilb                     | candela per square meter       | 0.318 309 9; $(1/\pi)$      |
|                              | lambert*                       | $10^{-4}$                   |
| Are                          | acre                           | 0.024 710 54                |
|                              | square meter*                  | 100                         |
| Assay ton                    | gram                           | 29.1667                     |
| Astronomical unit            | meter                          | $1.496\ 00 \times 10^{-11}$ |
|                              | light-year                     | $1.581\ 284 \times 10^{-5}$ |
| Atmosphere                   | bar*                           | 1.013 25.0                  |
|                              | foot of water (at 4°C)         | 33.898 54                   |
|                              | inch of mercury (at 0°C)       | 29.921 26                   |
|                              | kilogram per square centimeter | 1.033 227                   |
|                              | millimeter of mercury*         | 760                         |
|                              | millimeter of water (4°C)      | $1.033\ 227 \times 10^4$    |
|                              | newton per square meter*       | $1.013\ 250 \times 10^5$    |
|                              | pascal*                        | 101 325.0                   |
|                              | pound per square inch          | 14.695 95                   |
|                              | ton per square inch            | 0.007 348                   |
|                              | torr*                          | 760                         |
| Atomic mass unit             | gram                           | $1.6605 \times 10^{-24}$    |
| Avogadro number              | molecules per mole             | $6.022\ 137 \times 10^{23}$ |

TABLE 2.7 Conversion Factors (Continued)

| To convert                                 | Into                           | Multiply by                 |
|--------------------------------------------|--------------------------------|-----------------------------|
| Bar                                        | atmosphere                     | 0.986 923                   |
|                                            | dyne per square centimeter*    | $10^6$                      |
|                                            | kilogram per square centimeter | 1.019 716                   |
|                                            | millimeter of mercury          | 750.062                     |
|                                            | millimeter of water (4°C)      | $1.019\,716 \times 10^4$    |
|                                            | newton per square meter        | $10^5$                      |
|                                            | pascal*                        | $10^5$                      |
| Barn                                       | pound per square inch          | 14.503 77                   |
|                                            | square meter*                  | $10^{-28}$                  |
| Barrel (British)                           | gallon (British)*              | 36                          |
|                                            | liter                          | 163.659                     |
| Barrel (petroleum)                         | gallon (British)               | 34.9723                     |
|                                            | gallon (U.S.)*                 | 42                          |
| Barrel (U.S. dry)                          | liter                          | 158.987                     |
|                                            | bushel (U.S.)                  | 3.281 22                    |
|                                            | cubic foot                     | 4.083 33                    |
|                                            | liter                          | 115.6271                    |
| Barrel (U.S. liquid)                       | quart (U.S. dry)               | 104.9990                    |
|                                            | gallon (U.S.)                  | 31.5 (variable)             |
|                                            | liter                          | 119.2405                    |
| Barye                                      | dyne per square centimeter*    | 1                           |
| Becquerel                                  | curie*                         | $2.7 \times 10^{-11}$       |
| Biot                                       | ampere*                        | 10                          |
| Board foot                                 | cubic foot                     | (1/12)                      |
|                                            | cubic meter                    | $2.359\,737 \times 10^{-3}$ |
| Bohr                                       | meter                          | $5.291\,77 \times 10^{-11}$ |
| Bohr magneton                              | joule per tesla                | $9.274\,02 \times 10^{-24}$ |
| Bolt (U.S. cloth)                          | foot*                          | 120                         |
|                                            | meter                          | 36.576                      |
| Boltzmann constant                         | joule per degree               | $1.3806 \times 10^{-23}$    |
| British thermal unit (Btu)                 | calorie                        | 251.996                     |
|                                            | cubic foot-atmosphere          | 0.367 717                   |
|                                            | erg                            | $1.0550 \times 10^{10}$     |
|                                            | foot-pound                     | 778.169                     |
|                                            | horsepower-hour (British)      | $3.930\,15 \times 10^{-4}$  |
|                                            | horsepower-hour (metric)       | $3.984\,66 \times 10^{-4}$  |
|                                            | joule (International table)    | 1055.056                    |
|                                            | joule (thermochemical)         | 1054.350                    |
|                                            | kilogram-calorie               | 0.2520                      |
|                                            | kilogram-meter                 | 107.5                       |
|                                            | kilowatt-hour                  | $2.930\,71 \times 10^{-4}$  |
|                                            | liter-atmosphere               | 10.4126                     |
|                                            | kilocalorie per cubic meter    | 8.899 15                    |
| Btu per foot <sup>3</sup>                  | joule per meter <sup>3</sup>   | $3.725\,895 \times 10^4$    |
| Btu (International table)/ft <sup>3</sup>  | joule per meter <sup>3</sup>   | $3.723\,402 \times 10^4$    |
| Btu (thermochemical)/ft <sup>3</sup>       | watt                           | 0.293 071 1                 |
| Btu (International table)/hour             | watt                           | 0.292 875 1                 |
| Btu (thermochemical)/hour                  | joule per kilogram*            | $2.326 \times 10^3$         |
| Btu (thermochemical)/pound                 | joule per kilogram             | $2.324\,444 \times 10^3$    |
| Btu (thermochemical)/(ft <sup>2</sup> · h) | watt per meter <sup>2</sup>    | 3.154 591                   |
| Btu (thermochemical)/minute                | watt                           | 17.572 50                   |
| Btu (thermochemical)/pound                 | joule per kilogram             | $2.324\,444 \times 10^3$    |
| Btu per square foot                        | joule per square meter         | $1.135\,65 \times 10^4$     |
| Bucket (British, dry)                      | gallon (British)*              | 4                           |

**TABLE 2.7** Conversion Factors (*Continued*)

| To convert                     | Into                      | Multiply by                  |
|--------------------------------|---------------------------|------------------------------|
| Bushel (British)               | bushel (U.S.)             | 1.032 057                    |
|                                | cubic foot                | 1.284 35                     |
|                                | gallon (British)*         | 8                            |
|                                | gallon (U.S.)             | 9.607 60                     |
|                                | liter                     | 36.3687                      |
| Bushel (U.S.)                  | barrel (U.S., dry)        | 0.304 765                    |
|                                | bushel (British)          | 0.968 939                    |
|                                | cubic foot                | 1.244 456                    |
|                                | cubic meter               | 0.035 239 07                 |
|                                | gallon (British)          | 7.751 51                     |
|                                | gallon (U.S.)             | 9.309 18                     |
|                                | liter                     | 35.239 07                    |
|                                | peck (U.S.)*              | 4                            |
|                                | pint (U.S., dry)*         | 64                           |
|                                | foot                      | 607.611 55                   |
| Cable length (international)   | meter*                    | 185.2                        |
|                                | mile (nautical)*          | 0.1                          |
|                                | foot*                     | 720                          |
| Cable length (U.S. or British) | meter                     | 219.456                      |
|                                | mile (nautical)           | 0.118 407                    |
|                                | mile (statute)            | 0.136 364                    |
|                                | inch*                     | 0.01                         |
| Caliber                        | millimeter*               | 0.254                        |
|                                | Btu                       | 0.003 968 320                |
| Calorie                        | foot-pound                | 3.088 03                     |
|                                | foot-poundal              | 99.3543                      |
|                                | horsepower-hour (British) | $1.559\ 61 \times 10^{-6}$   |
|                                | joule*                    | 4.184                        |
|                                | kilowatt-hour             | $1.163 \times 10^{-6}$       |
|                                | liter-atmosphere          | 0.041 320 5                  |
|                                | joule                     | 4.1858                       |
| Calorie (15°C)                 | joule                     | 4.1868                       |
| Calorie (international)        | foot-pound per second     | 0.051 467 1                  |
| Calorie per minute             | horsepower (British)      | $9.357\ 65 \times 10^{-5}$   |
|                                | watt*                     | 0.069 78                     |
| Candela                        | Hefner unit               | 1.11                         |
|                                | lumen per steradian*      | 1                            |
| Candela per square centimeter  | candela per square foot*  | 929.0304                     |
|                                | candela per square meter* | $10^4$                       |
|                                | lambert                   | $3.141\ 593; (\pi)$          |
|                                | gram*                     | 0.2                          |
| Carat (metric)                 | Fahrenheit temperature    | $(9/5)^{\circ}\text{C} + 32$ |
| Celsius temperature            | kelvin                    | $^{\circ}\text{C} - 273.15$  |
| Centigrade heat unit or chu    | Btu*                      | 1.8                          |
|                                | calorie                   | 453.592                      |
|                                | joule                     | 1899.10                      |
| Centimeter                     | foot                      | 0.032 808 4                  |
|                                | inch                      | 0.393 700 8                  |
|                                | mil                       | 393.700 8                    |
| Centimeter of mercury (0°C)    | pascal                    | 1333.22                      |
| Centimeter of water (4°C)      | pascal                    | 98.063 8                     |
| Centimeter per second          | foot per minute           | 1.986 50                     |
|                                | kilometer per hour*       | 0.036                        |

TABLE 2.7 Conversion Factors (Continued)

| To convert                         | Into                         | Multiply by                |
|------------------------------------|------------------------------|----------------------------|
| Centimeter per second              | knot                         | 0.019 438 4                |
| (continued)                        | mile per hour                | 0.022 369 4                |
| Centimeter per second squared      | foot per second squared      | 0.032 808 4                |
|                                    | meter per second squared*    | 0.01                       |
| Centimeter-dyne                    | erg*                         | 1                          |
|                                    | joule*                       | $10^{-7}$                  |
|                                    | meter-kilogram               | $1.020 \times 10^{-8}$     |
|                                    | pound-foot                   | $7.376 \times 10^{-8}$     |
| Centimeter-gram                    | erg*                         | 980.665                    |
|                                    | joule*                       | $9.806\ 65 \times 10^{-5}$ |
| Centipoise                         | kilogram per (meter-second)* | 0.001                      |
|                                    | pascal-second*               | 0.001                      |
|                                    | pound per (foot-second)      | 0.006 72                   |
| Chain (Ramsden's)                  | foot*                        | 100                        |
|                                    | meter*                       | 30.48                      |
| Chain (Gunter's)                   | foot*                        | 66                         |
|                                    | meter*                       | 20.1168                    |
| Circular inch                      | circular mil*                | $10^6$                     |
|                                    | square centimeter            | 5.067 075                  |
|                                    | square inch                  | $(\pi/4)$                  |
| Circular millimeter                | square millimeter            | $(\pi/4)$                  |
| Circumference                      | degree*                      | 360                        |
|                                    | gon (grade)                  | 400                        |
|                                    | radian                       | $(2\pi)$                   |
| Cord                               | cord foot*                   | 8                          |
|                                    | cubic foot*                  | 128                        |
| Coulomb                            | ampere-second*               | 1                          |
| Coulomb per square centimeter      | coulomb per square inch*     | 6.4516                     |
| Cubic centimeter                   | cubic foot                   | $3.531\ 47 \times 10^{-5}$ |
|                                    | cubic inch                   | 0.061 023 744              |
|                                    | dram (U.S., fluid)           | 0.270 512 2                |
|                                    | gallon (British)             | $2.199\ 69 \times 10^{-4}$ |
|                                    | gallon (U.S.)                | $2.641\ 72 \times 10^{-4}$ |
|                                    | liter*                       | 0.001                      |
|                                    | minim (U.S.)                 | 16.230 73                  |
|                                    | ounce (British, fluid)       | 0.035 195 1                |
|                                    | ounce (U.S., fluid)          | 0.033 814 02               |
|                                    | pint (British)               | 0.001 759 75               |
|                                    | pint (U.S., dry)             | 0.001 816 17               |
|                                    | pint (U.S., liquid)          | 0.002 113 376              |
| Cubic centimeter-atmosphere        | joule*                       | 0.101 325                  |
|                                    | watt-hour                    | $2.814\ 58 \times 10^{-5}$ |
| Cubic centimeter per gram          | cubic foot per pound         | 0.016 018 5                |
| Cubic centimeter per second        | cubic foot per minute        | 0.002 118 88               |
|                                    | liter per hour*              | 3.6                        |
| Cubic decimeter (dm <sup>3</sup> ) | liter*                       | 1                          |
| Cubic foot                         | acre-foot                    | $2.295\ 68 \times 10^{-5}$ |
|                                    | board foot*                  | 12                         |
|                                    | cord*                        | (1/128)                    |
|                                    | cord foot*                   | (1/16)                     |
|                                    | cubic inch*                  | 1728                       |
|                                    | cubic meter*                 | 0.028 316 846 592          |
|                                    | cubic yard                   | (1/27)                     |

**TABLE 2.7** Conversion Factors (*Continued*)

| To convert                      | Into                                | Multiply by                 |
|---------------------------------|-------------------------------------|-----------------------------|
| Cubic foot ( <i>continued</i> ) | gallon (British)                    | 6.228 835                   |
|                                 | gallon (U.S.)                       | 7.480 519                   |
|                                 | liter                               | 28.316 847                  |
| Cubic foot per hour             | liter per minute                    | 0.471 947                   |
| Cubic foot per pound            | cubic meter per kilogram            | 0.062 428 0                 |
| Cubic foot-atmosphere           | Btu                                 | 2.719 48                    |
|                                 | calorie                             | 685.298                     |
|                                 | joule                               | 2869.205                    |
|                                 | kilogram-meter                      | 292.577                     |
|                                 | liter-atmosphere                    | 28.3168                     |
|                                 | watt-hour                           | 0.797 001                   |
|                                 | milliliter*                         | 16.387 064                  |
| Cubic inch                      | cubic foot                          | (1/1728)                    |
|                                 | milliliter*                         | 16.387 064                  |
| Cubic inch per minute           | cubic centimeter per second         | 0.273 118                   |
| Cubic kilometer                 | cubic mile                          | 0.239 913                   |
| Cubic meter per kilogram        | cubic foot per pound                | 16.0185                     |
| Cubic yard                      | bushel (British)                    | 21.0223                     |
|                                 | bushel (U.S.)                       | 21.6962                     |
|                                 | cubic foot*                         | 27                          |
|                                 | cubic meter                         | 0.764 554 86                |
|                                 | liter                               | 764.555                     |
| Cubic yard per minute           | cubic foot per second*              | 0.45                        |
|                                 | gallon (British) per second         | 2.802 98                    |
|                                 | gallon (U.S.) per second            | 3.366 23                    |
|                                 | liter per second                    | 12.742 58                   |
|                                 | inch*                               | 18                          |
| Cubit                           | inch*                               | 18                          |
| Cup (U.S.)                      | milliliter; centimeter <sup>3</sup> | 236.6                       |
| Cup (metric)                    | cubic centimeter*                   | 200                         |
| Curie                           | becquerel*                          | $3.7 \times 10^{10}$        |
| Cycle per second                | hertz*                              | 1                           |
| Dalton                          | kilogram                            | $1.660\ 54 \times 10^{-27}$ |
|                                 | unified atomic mass*                | 1                           |
| Day (mean solar)                | hour*                               | 24                          |
|                                 | minute*                             | 1440                        |
|                                 | second*                             | 86 400                      |
|                                 | coulomb-meter                       | $3.335\ 64 \times 10^{-30}$ |
| Debye                           | coulomb-meter                       | $3.335\ 64 \times 10^{-30}$ |
| Decibel                         | neper                               | 0.115 129 255               |
| Degree (plane angle)            | circumference                       | (1/366)                     |
|                                 | gon (grade)                         | 1.111 11                    |
|                                 | minute (angle)*                     | 60                          |
|                                 | quadrant                            | (1/90)                      |
|                                 | radian                              | ( $\pi$ /180)               |
|                                 | revolution                          | (1/360)                     |
|                                 | second (angle)*                     | 3600                        |
|                                 | radian per meter                    | 0.057 261 5                 |
| Degree (angle) per foot         | radian per second                   | 0.017 453 3                 |
| Degree (angle) per second       | degree Fahrenheit*                  | 1.8                         |
| Degree Celsius                  | degree Rankine*                     | 1.8                         |
|                                 | kelvin*                             | 1                           |
|                                 | degree Celsius                      | (5/9)                       |
| Degree Fahrenheit               | kelvin                              | (5/9)                       |
| Degree Rankine                  | tex                                 | (1/9)                       |
| Denier                          | coulomb-meter                       | $1.602\ 18 \times 10^{-21}$ |
| Dipole length ( <i>e</i> cm)    | coulomb-meter                       | $1.602\ 18 \times 10^{-21}$ |

TABLE 2.7 Conversion Factors (Continued)

| To convert                              | Into                           | Multiply by                 |
|-----------------------------------------|--------------------------------|-----------------------------|
| Drachm (British)                        | dram (apothecaries or troy)*   | 1                           |
| Drachm (British, fluid)                 | cubic centimeter               | 3.551 633                   |
|                                         | dram (U.S., fluid)             | 0.960 760                   |
|                                         | minim (British)                | 60                          |
|                                         | ounce (British, fluid)         | (1/8)                       |
| Dram (apothecaries or troy)             | dram (weight)                  | 2.194 285 7                 |
|                                         | grain*                         | 60                          |
|                                         | gram*                          | 3.887 934 6                 |
|                                         | ounce (troy)*                  | (1/8)                       |
|                                         | pennyweight*                   | 2.5                         |
|                                         | pound (troy)*                  | (1/96)                      |
|                                         | scruple*                       | 3                           |
|                                         | grain*                         | 27.343 75                   |
| Dram (weight)                           | gram                           | 1.771 845 2                 |
|                                         | ounce (weight)                 | (1/16)                      |
|                                         | pound (weight)                 | (1/256)                     |
| Dram (U.S., fluid)                      | cubic centimeter               | 3.696 691 2                 |
|                                         | gallon (U.S.)                  | (1/1024)                    |
|                                         | gill (U.S.)                    | (1/32)                      |
|                                         | milliliter                     | 3.696 691 2                 |
|                                         | minim (U.S.)*                  | 60                          |
|                                         | ounce (U.S., fluid)            | (1/8)                       |
|                                         | pint (U.S., fluid)             | (1/128)                     |
| Dyne                                    | kilogram (force)               | $1.019\,716 \times 10^{-6}$ |
|                                         | newton*                        | $10^{-5}$                   |
|                                         | pound (force)                  | $2.248\,09 \times 10^{-6}$  |
|                                         | newton per meter*              | 0.001                       |
| Dyne per centimeter                     | bar*                           | $10^{-6}$                   |
| Dyne per square centimeter              | kilogram per square centimeter | $1.019\,716 \times 10^{-6}$ |
|                                         | millimeter of mercury (0°C)    | $7.500\,617 \times 10^{-4}$ |
|                                         | millimeter of water (4°C)      | 0.010 197 16                |
|                                         | newton per square meter*       | 0.1                         |
|                                         | pascal*                        | 0.1                         |
|                                         | pound per square inch (psi)    | $1.450\,38 \times 10^{-5}$  |
| Dyne-centimeter                         | erg*                           | 1                           |
|                                         | foot-pound (force)             | $7.375\,62 \times 10^{-8}$  |
|                                         | foot-poundal                   | $2.373\,04 \times 10^{-6}$  |
|                                         | joule*                         | $10^{-7}$                   |
|                                         | kilogram-meter (force)         | $1.019\,716 \times 10^{-8}$ |
|                                         | newton-meter*                  | $10^{-7}$                   |
| Dyne-second/centimeter <sup>2</sup>     | poise*                         | 1                           |
|                                         | pascal-second*                 | 0.1                         |
| Electron charge                         | coulomb                        | $1.602\,18 \times 10^{-19}$ |
| Electron charge-centimeter<br>(e cm)    | coulomb-meter                  | $1.602\,18 \times 10^{-21}$ |
| Electron charge-centimeter <sup>2</sup> | coulomb-meter squared          | $1.602\,18 \times 10^{-23}$ |
| Electron mass                           | atomic mass unit               | 0.000 548 6                 |
|                                         | gram                           | $9.1096 \times 10^{-28}$    |
| Electronvolt                            | erg                            | $1.602\,18 \times 10^{-12}$ |
|                                         | joule                          | $1.602\,18 \times 10^{-19}$ |
|                                         | kilojoule per mole             | 96.4853                     |
|                                         | inch*                          | 45                          |
| Ell                                     | inch                           | 0.167                       |
| Em, pica                                | millimeter                     | 4.217 52                    |



**TABLE 2.7** Conversion Factors (*Continued*)

| To convert                         | Into                          | Multiply by                  |
|------------------------------------|-------------------------------|------------------------------|
| EMU <sup>1</sup> of capacitance    | farad*                        | 10 <sup>9</sup>              |
| EMU of current                     | ampere*                       | 10                           |
| EMU of electric potential          | volt*                         | 10 <sup>-8</sup>             |
| EMU of inductance                  | henry*                        | 10 <sup>-9</sup>             |
| EMU of quantity (charge)           | coulomb                       | 10                           |
| EMU of resistance                  | ohm                           | 10 <sup>-9</sup>             |
| EMU of work                        | joule                         | 10 <sup>-7</sup>             |
| ESU <sup>2</sup> of capacitance    | farad                         | $1.112\ 650 \times 10^{-12}$ |
| ESU of current                     | ampere                        | $3.335\ 641 \times 10^{-10}$ |
| ESU of electric potential          | volt                          | 299.792 5                    |
| ESU of inductance                  | henry                         | $8.987\ 552 \times 10^{11}$  |
| ESU of quantity (charge)           | coulomb                       | $3.335\ 556 \times 10^{-11}$ |
| ESU of resistance                  | ohm                           | $8.987\ 552 \times 10^{11}$  |
| ESU of work                        | joule                         | 10 <sup>-7</sup>             |
| Erg                                | dyne-centimeter*              | 1                            |
|                                    | joule*                        | 10 <sup>-7</sup>             |
|                                    | watt-hour                     | $2.777\ 78 \times 10^{-11}$  |
| Erg per second                     | Btu                           | $5.69 \times 10^{-6}$        |
|                                    | watt*                         | 10 <sup>-7</sup>             |
| Erg per (cm <sup>2</sup> × second) | watt per square meter*        | 0.001                        |
| Erg per gauss                      | ampere-centimeter squared*    | 10                           |
|                                    | joule per tesla*              | 0.001                        |
| Fahrenheit scale                   | centigrade scale              | (5/9)                        |
| Fahrenheit temperature (°F)        | Celsius temperature (°C)      | (°F - 32)/(5/9)              |
| Faraday (based on carbon-12)       | coulomb                       | 96 487.0                     |
| Faraday (chemical)                 | coulomb                       | 96 495.7                     |
| Faraday (physical)                 | coulomb                       | 96 521.9                     |
| Fathom                             | foot*                         | 6                            |
|                                    | meter                         | 1.828 8                      |
| Fermi                              | meter*                        | 10 <sup>-15</sup>            |
| Foot                               | centimeter*                   | 30.48                        |
|                                    | inch*                         | 12                           |
|                                    | mile (nautical)               | $1.645\ 788 \times 10^{-4}$  |
|                                    | mile (statute)                | $1.893\ 939 \times 10^{-4}$  |
|                                    | yard                          | (1/3)                        |
| Foot of water (4°C)                | atmosphere                    | 0.029 499 8                  |
|                                    | bar                           | 0.029 499 8                  |
|                                    | gram per square centimeter    | 30.48                        |
|                                    | inch of mercury (0°C)         | 0.882 671                    |
|                                    | pascal                        | 2989.067                     |
| Foot per minute                    | centimeter per second*        | 0.508                        |
|                                    | knot                          | 0.009 874 73                 |
|                                    | mile per hour                 | 0.011 363 6                  |
| Foot-candle                        | lumen per square foot*        | 1                            |
|                                    | lumen per square meter        | 10.7639                      |
|                                    | lux                           | 10.76391                     |
| Foot-lambert                       | candela per square centimeter | $3.426\ 26 \times 10^{-4}$   |
|                                    | candela per square foot       | (1/π)                        |
|                                    | lambert                       | 0.001 076 39                 |
|                                    | meter-lambert                 | 10.7639                      |

<sup>1</sup> EMU, the electromagnetic system of electrical units based on dynamics.<sup>2</sup> ESU, the electrostatic system of electrical units based on static data.

TABLE 2.7 Conversion Factors (Continued)

| To convert                   | Into                             | Multiply by                 |
|------------------------------|----------------------------------|-----------------------------|
| Foot-pound                   | Btu                              | 0.001 285 07                |
|                              | calorie                          | 0.323 832                   |
|                              | foot-poundal                     | 32.1740                     |
|                              | horsepower (British)             | $5.050\ 51 \times 10^{-7}$  |
|                              | joule                            | 1.355 818                   |
|                              | kilogram-meter                   | 0.138 255                   |
|                              | liter-atmosphere                 | 0.013 380 9                 |
|                              | newton-meter                     | 1.355 818                   |
|                              | watt-hour                        | $3.766\ 161 \times 10^{-4}$ |
| Foot-pound per minute        | horsepower (British)             | $3.030\ 30 \times 10^{-5}$  |
|                              | horsepower (metric)              | $3.072\ 33 \times 10^{-5}$  |
|                              | watt                             | 0.022 597 0                 |
| Foot-poundal                 | Btu                              | $3.994\ 11 \times 10^{-5}$  |
|                              | calorie                          | 0.010 064 99                |
|                              | foot-pound                       | 0.031 081 0                 |
|                              | joule                            | 0.042 140 11                |
|                              | kilogram-meter                   | 0.004 297 10                |
|                              | liter-atmosphere                 | $4.158\ 91 \times 10^{-4}$  |
|                              | watt-hour                        | $1.170\ 56 \times 10^{-5}$  |
|                              | coulomb                          | $3.335\ 64 \times 10^{-10}$ |
| Franklin                     | coulomb per cubic meter          | $3.335\ 64 \times 10^{-4}$  |
| Franklin per cm <sup>3</sup> | coulomb per square meter         | $3.335\ 64 \times 10^{-6}$  |
| Franklin per cm <sup>2</sup> | chain (Gunter's)*                | 10                          |
| Furlong                      | foot*                            | 600                         |
|                              | meter*                           | 201.168                     |
|                              | mile                             | (1/8)                       |
|                              | bushel (British)                 | (1/8)                       |
|                              | cubic decimeter, liter*          | 4.546 90                    |
|                              | cubic foot                       | 0.160 544                   |
|                              | gallon (U.S., fluid)             | 1.200 95                    |
|                              | gill (British)*                  | 32                          |
| Gallon (British, imperial)   | liter                            | 4.546 09                    |
|                              | ounce (British)*                 | 160                         |
|                              | quart (British)*                 | 4                           |
|                              | barrel (petroleum)               | (1/42)                      |
|                              | cubic decimeter, liter           | 3.785 41                    |
|                              | cubic foot                       | 0.133 680 56                |
|                              | gallon (British)                 | 0.832 674                   |
|                              | liter                            | 3.785 41                    |
| Gallon (U.S.)                | ounce (U.S., fluid)*             | 128                         |
|                              | quart (U.S., fluid)*             | 4                           |
|                              | cubic foot per hour              | 8.020 83                    |
|                              | cubic meter per hour             | 0.227 125                   |
|                              | liter per minute                 | 3.785 412                   |
| Gamma                        | microgram*                       | 1                           |
| Gas constant                 | calorie per mole-degree          | 1.987                       |
|                              | joule per mole-degree            | 8.3143                      |
|                              | liter-atmosphere per mole-degree | 0.082 057                   |
|                              |                                  |                             |
| Gauss                        | tesla*                           | 10 <sup>-4</sup>            |
|                              | weber per square meter*          | 10 <sup>-4</sup>            |
| Gilbert                      | ampere-turn                      | 0.795 775                   |

TABLE 2.7 Conversion Factors (Continued)

| To convert                 | Into                    | Multiply by                   |
|----------------------------|-------------------------|-------------------------------|
| Gill (British)             | cubic centimeter, mL    | 142.065                       |
|                            | cubic inch              | 8.669 36                      |
|                            | gallon (British)        | (1/32)                        |
|                            | gill (U.S.)             | 1.200 95                      |
|                            | ounce (British, fluid)* | 5                             |
|                            | pint (British)          | (1/4)                         |
| Gill (U.S.)                | cubic centimeter, mL    | 118.2941                      |
|                            | gallon (U.S.)           | (1/32)                        |
|                            | liter                   | 0.118 294 1                   |
|                            | ounce (U.S., fluid)*    | 4                             |
|                            | quart (U.S.)            | (1/8)                         |
|                            | circumference           | (1/400)                       |
| Gon (grade)                | minute (angle)*         | 54                            |
|                            | radian                  | (2 $\pi$ /400)                |
|                            | radian                  | (2 $\pi$ /400)                |
| Grade                      | carat (metric)*         | 0.323 994 55                  |
|                            | milligram*              | 64.798 91                     |
|                            | ounce (weight)          | 0.002 285 714 3               |
|                            | ounce (troy)            | (1/480)                       |
|                            | pennyweight             | (1/24)                        |
|                            | pound                   | (1/7000)                      |
|                            | scruple                 | (1/20)                        |
| Gram                       | carat (metric)*         | 5                             |
|                            | dram                    | 0.564 383 39                  |
|                            | grain                   | 15.432 358                    |
|                            | ounce (weight)          | 0.035 273 962                 |
|                            | ounce (troy)            | 0.032 150 747                 |
|                            | pennyweight             | 0.643 014 93                  |
|                            | pound                   | 0.002 204 622 6               |
|                            | ton (metric)*           | 10 <sup>-6</sup>              |
|                            | poise*                  | 1                             |
|                            | kilogram per liter*     | 1                             |
| Gram per cubic centimeter  | pound per cubic foot    | 62.4280                       |
|                            | pound per gallon (U.S.) | 8.345 40                      |
|                            | ounce per square foot   | 0.327 706                     |
| Gram per square meter      | gram per ton (metric)   | 0.984 207                     |
| Gram per ton (long)        | gram per ton (short)    | 0.892 857                     |
|                            | dyne*                   | 980.665                       |
| Gram (force)               | newton*                 | 0.009 806 65                  |
|                            | pascal*                 | 98.0665                       |
| Gram per square centimeter | joule*                  | 9.806 65 $\times 10^{-5}$     |
| Gram-centimeter            | pound-square foot       | 2.373 04 $\times 10^{-6}$     |
| Gram-square centimeter     | joule per kilogram*     | 1                             |
| Gray                       | electron volt           | 27.211 40                     |
| Hartree                    | hertz                   | 6.579 683 90 $\times 10^{15}$ |
|                            | joule                   | 4.359 75 $\times 10^{-18}$    |
|                            | acre                    | 2.471 054                     |
|                            | are*                    | 100                           |
| Hectare                    | meter squared           | 10 <sup>4</sup>               |
|                            | candela                 | 0.9                           |
| Hefner unit                | sphere*                 | 0.5                           |
| Hemisphere                 | spherical right angle*  | 4                             |
|                            | steradian               | (2 $\pi$ )                    |

TABLE 2.7 Conversion Factors (Continued)

| To convert                | Into                                    | Multiply by                 |
|---------------------------|-----------------------------------------|-----------------------------|
| Hertz                     | cycle per second*                       | 1                           |
| Hogshead                  | gallon (U.S.)*                          | 63                          |
| Horsepower (British)      | Btu per hour                            | 2544.43                     |
|                           | foot pound per hour*                    | $1.98 \times 10^6$          |
|                           | horsepower (metric)                     | 1.013 87                    |
|                           | joule per second                        | 745.700                     |
|                           | kilocalorie per hour                    | 641.186                     |
|                           | kilogram-meter per second               | 76.0402                     |
|                           | watt                                    | 745.70                      |
| Horsepower (electric)     | watt*                                   | 746                         |
| Horsepower-hour (British) | Btu                                     | 2544.43                     |
|                           | foot-pound*                             | $1.98 \times 10^6$          |
|                           | joule                                   | $2.684\ 52 \times 10^6$     |
|                           | kilocalorie                             | 641.186                     |
|                           | kilogram-meter                          | $2.737\ 45 \times 10^5$     |
|                           | watt-hour                               | 745.7                       |
| Hour (mean solar)         | day                                     | (1/24)                      |
|                           | minute*                                 | 60                          |
|                           | second*                                 | 3600                        |
|                           | week                                    | (1/168)                     |
| Hundredweight (long)      | kilogram*                               | 50.802 345 44               |
|                           | pound*                                  | 112                         |
|                           | ton (long)                              | (1/20)                      |
|                           | ton (metric)                            | 0.050 802 345               |
|                           | ton (short)*                            | 0.056                       |
| Hundredweight (short)     | hundredweight (long)                    | 0.892 857                   |
| Inch                      | centimeter*                             | 2.54                        |
|                           | foot                                    | (1/12)                      |
|                           | mil*                                    | 1000                        |
|                           | atmosphere                              | 0.033 421 05                |
| Inch of mercury (0°C)     | inch of water (4°C)                     | 13.5951                     |
|                           | millibar                                | 33.863 88                   |
|                           | millimeter of water (4°C)               | 345.316                     |
|                           | pascal                                  | 3386.388                    |
|                           | pound per square inch, psi              | 0.491 1541                  |
|                           | inch of mercury (0°C)                   | 0.073 5559                  |
|                           | millibar                                | 2.490 89                    |
| Inch of water (4°C)       | millimeter of mercury (0°C)             | 1.868 32                    |
|                           | pascal                                  | 249.089                     |
|                           | pound per square inch, psi              | 0.036 1273                  |
| Inch per minute           | foot per hour*                          | 5                           |
|                           | meter per hour*                         | 1.524                       |
|                           | millimeter per second                   | 0.423 333                   |
|                           | Btu                                     | $9.478\ 170 \times 10^{-4}$ |
| Joule                     | calorie*                                | 0.2390                      |
|                           | centigrade heat unit, chu               | 5.265 65                    |
|                           | centimeter-dyne*                        | $10^7$                      |
|                           | cubic foot-atmosphere                   | 0.000 348 529               |
|                           | cubic foot-(pound per in <sup>2</sup> ) | 0.005 121 959               |
|                           | erg*                                    | $10^7$                      |
|                           | foot-pound                              | 0.737 562                   |
|                           | foot-poundal                            | 23.7304                     |
|                           | horsepower-hour (British)               | $3.725\ 06 \times 10^{-7}$  |
|                           | liter-atmosphere                        | 0.009 869 233               |

**TABLE 2.7** Conversion Factors (*Continued*)

| To convert                 | Into                                 | Multiply by                          |
|----------------------------|--------------------------------------|--------------------------------------|
| Joule ( <i>continued</i> ) | newton-meter*                        | 1                                    |
|                            | watt-second*                         | 1                                    |
| Joule per centimeter       | kilogram (force)                     | 10.197 16                            |
|                            | newton*                              | 100                                  |
|                            | pound (force)                        | 22.4809                              |
| Joule per gram             | Btu per pound                        | 0.429 923                            |
|                            | kilocalorie per kilogram             | 0.238 846                            |
|                            | watt-hour per pound                  | 0.125 998                            |
| Joule per second           | watt*                                | 1                                    |
| Kilogram (force)           | dyne*                                | 9.806 65 $\times 10^5$               |
|                            | newton*                              | 9.806 65                             |
|                            | pound (force)                        | 2.204 62                             |
|                            | poundal                              | 70.9316                              |
| Kilometer                  | astronomical unit                    | 6.684 59 $\times 10^{-9}$            |
|                            | mile (nautical)                      | 0.539 956 80                         |
|                            | mile (statute)                       | 0.621 371 192                        |
| Kilowatt                   | Btu per minute                       | 56.8690                              |
|                            | foot-pound per second                | 737.562                              |
|                            | horsepower (British)                 | 1.341 02                             |
|                            | horsepower (metric)                  | 1.359 62                             |
|                            | joule per second*                    | 1000                                 |
|                            | kilocalorie per hour                 | 859.845                              |
| Kilowatt-hour              | Btu                                  | 3412.14                              |
|                            | horsepower-hour (British)            | 1.341 02                             |
|                            | joule*                               | 3.6 $\times 10^6$                    |
|                            | kilocalorie                          | 859.845                              |
| Knot                       | foot per minute                      | 101.2686                             |
|                            | kilometer per hour*                  | 1.852                                |
|                            | mile (nautical) per hour*            | 1                                    |
|                            | mile (statute) per hour              | 1.150 78                             |
| Lambda                     | decimeter cubed*                     | 10 <sup>-6</sup>                     |
|                            | microliter*                          | 1                                    |
| Lambert                    | candela per square meter             | (1/ $\pi$ ) $\times 10^4$ ; 3183.099 |
|                            | candela per square inch              | 2.053 61                             |
|                            | foot-lambert                         | 929.030                              |
| Langley                    | joule per square meter*              | 4.184 $\times 10^4$                  |
| League (nautical)          | mile (nautical)*                     | 3                                    |
| League (statute)           | mile (statute)*                      | 3                                    |
| Light-year                 | astronomical unit                    | 6.323 97 $\times 10^4$               |
|                            | meter                                | 9.460 73 $\times 10^{15}$            |
| Link                       | chain*                               | 0.01                                 |
| Liter                      | cubic decimeter (dm <sup>3</sup> )*  | 1                                    |
|                            | cubic foot                           | 0.035 314 67                         |
|                            | gallon (British)                     | 0.219 969                            |
|                            | gallon (U.S.)                        | 0.264 172 1                          |
|                            | quart (British)                      | 0.879 877                            |
|                            | quart (U.S.)                         | 1.056 688                            |
| Liter per minute           | cubic foot per hour                  | 2.118 88                             |
|                            | gallon (British) per hour            | 13.198                               |
|                            | gallon (U.S.) per hour               | 15.8503                              |
| Liter-atmosphere           | Btu                                  | 0.096 037 6                          |
|                            | calorie                              | 24.2011                              |
|                            | cubic foot-atmosphere                | 0.035 314 7                          |
|                            | cubic foot-pound per in <sup>2</sup> | 0.518 983                            |

TABLE 2.7 Conversion Factors (Continued)

| To convert                   | Into                        | Multiply by                 |
|------------------------------|-----------------------------|-----------------------------|
| Liter-atmosphere (continued) | horsepower (British)        | $3.774\ 42 \times 10^{-5}$  |
|                              | horsepower (metric)         | $3.826\ 77 \times 10^{-5}$  |
|                              | joule*                      | 101.325                     |
|                              | kilogram-meter              | 10.332 27                   |
|                              | watt-hour                   | 0.028 145 8                 |
| Lumen per square centimeter  | lux*                        | $10^4$                      |
|                              | phot*                       | 1                           |
| Lumen per square meter       | lumen per square foot       | 0.092 903 0                 |
| Lux                          | lumen per square meter*     | 1                           |
| Maxwell                      | weber*                      | $10^{-8}$                   |
| Meter                        | ångström*                   | $10^{10}$                   |
|                              | fathom                      | 0.546 807                   |
|                              | foot                        | 3.280 839 895               |
|                              | inch                        | 39.370 078 740              |
|                              | mile (nautical)             | $5.399\ 568 \times 10^{-4}$ |
|                              | mile (statute)              | $6.213\ 712 \times 10^{-4}$ |
|                              | foot per minute             | 196.850                     |
|                              | kilometer per hour*         | 3.6                         |
|                              | knot                        | 1.943 844                   |
| Meter per second             | mile per hour               | 2.236 936                   |
|                              | lux*                        | 1                           |
| Meter-candle                 |                             |                             |
| Meter-lambert                | candela per square meter    | $(1/\pi)$                   |
|                              | foot-lambert                | 0.092 903 0                 |
|                              | lambert*                    | $10^{-4}$                   |
| Mho (ohm <sup>-1</sup> )     | siemen*                     | 1                           |
| Micron                       | meter                       | $10^{-6}$                   |
| Mil                          | inch*                       | 0.001                       |
|                              | micrometer*                 | 25.4                        |
| Mile (nautical)              | foot                        | 6076.115 49                 |
|                              | kilometer*                  | 1.852                       |
|                              | mile (statute)              | 1.150 78                    |
| Mile (statute)               | chain (Gunter's)*           | 80                          |
|                              | chain (Ramsden's)*          | 52.8                        |
|                              | foot*                       | 5280                        |
|                              | furlong*                    | 8                           |
|                              | kilometer*                  | 1.609 344                   |
|                              | light-year                  | $1.701\ 11 \times 10^{-11}$ |
|                              | link (Gunter's)*            | 8000                        |
|                              | link (Ramsden's)*           | 5280                        |
|                              | mile (nautical)             | 0.868 976                   |
| Mile per gallon (British)    | rod*                        | 320                         |
|                              | kilometer per liter         | 0.354 006                   |
| Mile per gallon (U.S.)       | kilometer per liter         | 0.425 144                   |
| Mile per hour                | foot per minute             | 88                          |
|                              | kilometer per hour*         | 1.609 344                   |
|                              | knot                        | 0.868 976                   |
| Milliliter                   | cubic centimeter*           | 1                           |
| Millimeter of mercury (0°C)  | atmosphere                  | (1/760)                     |
|                              | dyne per square centimeter  | 1333.224                    |
|                              | millimeter of water (4°C)   | 13.5951                     |
|                              | pascal                      | 133.322                     |
|                              | pound per square inch (psi) | 0.019 336 8                 |
|                              | torr*                       | 1                           |

TABLE 2.7 Conversion Factors (Continued)

| To convert                    | Into                           | Multiply by                 |
|-------------------------------|--------------------------------|-----------------------------|
| Millimeter of water (4°C)     | atmosphere                     | 0.009 678 41                |
|                               | millibar*                      | 0.098 066 5                 |
|                               | millimeter of mercury (0°C)    | 0.073 555 9                 |
|                               | pascal*                        | 9.806 65                    |
|                               | pound per square inch          | 0.001 422 33                |
| Minim (British)               | milliliter                     | 0.059 193 9                 |
|                               | minim (U.S.)                   | 0.960 760                   |
| Minim (U.S.)                  | milliliter                     | 0.061 611 5                 |
| Minute (plane angle)          | circumference                  | $4.629\ 63 \times 10^{-5}$  |
|                               | degree (angle)                 | (1/60)                      |
|                               | gon                            | (1/54)                      |
|                               | radian                         | ( $\pi$ /10,800)            |
| Minute                        | hour                           | (1/60)                      |
|                               | second                         | 60                          |
| Month (mean of 4-year period) | day                            | 30.4375                     |
|                               | hour                           | 730.5                       |
|                               | week                           | 4.348 21                    |
| Nail (British)                | inch*                          | 2.25                        |
| Nanometer                     | ångström*                      | 10                          |
| Neper                         | decibel                        | 8.685 890                   |
| Nuclear magneton              | joule per tesla                | $5.050\ 79 \times 10^{-27}$ |
| Neutron mass                  | atomic mass unit               | 1.008 66                    |
|                               | gram                           | $1.6749 \times 10^{-24}$    |
|                               | dyne*                          | $10^5$                      |
| Newton                        | kilogram (force)               | 0.101 971 6                 |
|                               | pound (force)                  | 0.224 809                   |
|                               | poundal                        | 7.233 01                    |
|                               | See pascal                     |                             |
| Newton per square meter       | foot-pound                     | 0.737 562                   |
| Newton-meter                  | joule*                         | 1                           |
|                               | kilogram-meter                 | 0.101 971 6                 |
|                               | watt-second*                   | 1                           |
|                               | candela per square meter*      | 1                           |
| Nit                           | gill (British)*                | 1                           |
| Noggin (British)              | lux*                           | 0.001                       |
| Nox                           | ampere per meter (in practice) | (1000/4 $\pi$ ); 79.577 47  |
| Oersted                       | ohm                            | 1.000 49                    |
| Ohm (mean international)      | ohm                            | 1.000 495                   |
| Ohm (U.S. international)      | ohm per meter                  | 3.280 84                    |
| Ohm per foot                  | dram*                          | 16                          |
|                               | grain*                         | 437.5                       |
|                               | gram*                          | 28.349 5                    |
|                               | ounce (troy)                   | 0.911 458 33                |
|                               | pound                          | (1/16)                      |
| Ounce (troy)                  | grain*                         | 480                         |
|                               | gram*                          | 31.1035                     |
|                               | ounce (avoirdupois)            | 1.097 142 9                 |
|                               | pennyweight*                   | 20                          |
|                               | pound (avoirdupois)            | 0.068 571 429               |
|                               | scruple*                       | 24                          |
| Ounce (British, fluid)        | cubic centimeter               | 28.413 06                   |
|                               | gallon (British)               | (1/160)                     |
|                               | milliliter                     | 28.413 06                   |

TABLE 2.7 Conversion Factors (Continued)

| To convert                            | Into                        | Multiply by                  |
|---------------------------------------|-----------------------------|------------------------------|
| Ounce (British, fluid)<br>(continued) | minim (British)             | 480                          |
|                                       | ounce (U.S., fluid)         | 0.960 760                    |
|                                       | pint (British)              | (1/20)                       |
|                                       | quart (British)             | (1/40)                       |
| Ounce (U.S., fluid)                   | cubic centimeter            | 29.573 530                   |
|                                       | gallon (U.S.)               | (1/128)                      |
|                                       | milliliter                  | 29.573 530                   |
|                                       | pint (U.S., fluid)          | (1/16)                       |
|                                       | quart (U.S., fluid)         | (1/32)                       |
| Ounce (avoirdupois) per cubic foot    | kilogram per cubic meter    | 1.001 154                    |
| Ounce (avoirdupois)/gallon (U.S.)     | gram per liter              | 7.489 15                     |
| Ounce (avoirdupois) per ton (long)    | gram per ton (metric)       | 27.9018                      |
| Ounce (avoirdupois) per ton (short)   | milligram per kilogram      | 27.9018                      |
|                                       | gram per ton (metric)*      | 31.25                        |
|                                       | milligram per kilogram*     | 31.25                        |
| Parsec                                | light-year                  | 3.261 636                    |
| Part per million                      | milligram per kilogram*     | 1                            |
| Pascal                                | milliliter per cubic meter* | 1                            |
|                                       | atmosphere                  | 9.869 233 × 10 <sup>-6</sup> |
|                                       | bar*                        | 10 <sup>-5</sup>             |
|                                       | dyne per square centimeter* | 10                           |
|                                       | inch of mercury             | 2.953 00 × 10 <sup>-4</sup>  |
|                                       | millimeter of mercury       | 7.500 62 × 10 <sup>-3</sup>  |
|                                       | millimeter of water         | 0.101 972                    |
|                                       | newton per square meter*    | 1                            |
|                                       | pound per square inch       | 1.450 377 × 10 <sup>-4</sup> |
|                                       | poundal per square foot     | 0.671 969                    |
| Pascal-second                         | poise*                      | 10                           |
| Peck (British)                        | gallon (British)*           | 2                            |
| Peck (U.S.)                           | bushel (U.S.)*              | 0.25                         |
| Pennyweight                           | grain*                      | 24                           |
|                                       | gram*                       | 1.555 173 84                 |
|                                       | ounce (troy)                | (1/20)                       |
|                                       | pound                       | 0.003 428 571 4              |
|                                       | lux*                        | 10 <sup>4</sup>              |
| Phot                                  |                             |                              |
| Pica (printer's)                      | inch                        | 0.167                        |
|                                       | point*                      | 12                           |
| Pint (British)                        | gallon (British)            | (1/8)                        |
|                                       | liter                       | 0.568 261                    |
|                                       | pint (U.S., fluid)          | 1.200 95                     |
|                                       | quart (British)             | 0.5                          |
| Pint (U.S., dry)                      | bushel (U.S.)               | (1/64)                       |
|                                       | liter                       | 0.550 610 5                  |
|                                       | peck (U.S.)                 | (1/16)                       |
|                                       | pint (British)              | 0.968 939                    |
|                                       | quart (U.S., dry)           | 0.5                          |
| Pint (U.S., fluid)                    | gallon (U.S.)               | (1/8)                        |
|                                       | liter                       | 0.473 176 5                  |



**TABLE 2.7** Conversion Factors (*Continued*)

| To convert                                             | Into                                      | Multiply by                    |
|--------------------------------------------------------|-------------------------------------------|--------------------------------|
| Pint (U.S., fluid)                                     | pint (British)                            | 0.832 674                      |
| ( <i>continued</i> )                                   | quart (U.S., fluid)*                      | 0.5                            |
| Planck's constant                                      | joule-second                              | $6.626\ 08 \times 10^{-34}$    |
| Point (printer's, Didot)                               | millimeter                                | 0.376 065 03                   |
| Point (printer's, U.S.)                                | millimeter*                               | 0.351 459 8                    |
| Poise                                                  | dyne-second per square centimeter*        | 1                              |
|                                                        | pascal-second*                            | 0.1                            |
| Polarizability volume ( $4\pi\epsilon_0\text{ cm}^3$ ) | coulomb squared-(meter squared per joule) | $1.112\ 65 \times 10^{-16}$    |
| Pole (British)                                         | foot*                                     | 16.5                           |
| Pottle (British)                                       | gallon (British)*                         | 0.5                            |
| Pound                                                  | gram*                                     | 453.592 37                     |
|                                                        | ounce (weight)*                           | 16                             |
|                                                        | ton (long)                                | $4.464\ 285\ 7 \times 10^{-4}$ |
|                                                        | ton (short)                               | (1/2000)                       |
| Pound (troy)                                           | grain                                     | 5760                           |
|                                                        | gram*                                     | 373.241 721 6                  |
|                                                        | ounce (troy)*                             | 12                             |
|                                                        | pennyweight                               | 240                            |
|                                                        | pound (weight)                            | 0.822 857 14                   |
|                                                        | scruple*                                  | 288                            |
| Pound per cubic foot                                   | kilogram per cubic meter                  | 16.018 46                      |
| Pound per cubic inch                                   | gram per cubic centimeter                 | 27.679 905                     |
|                                                        | pound per cubic foot*                     | 1728                           |
| Pound per foot                                         | kilogram per meter                        | 1.488 16                       |
| Pound per (foot-second)                                | pascal-second                             | 1.488 16                       |
| Pound per gallon (U.S.)                                | gram per liter                            | 119.8264                       |
| Pound per hour                                         | kilogram per day                          | 10.886 22                      |
| Pound per inch                                         | kilogram per meter                        | 17.857 97                      |
| Pound per minute                                       | kilogram per hour                         | 27.215 54                      |
| Pound per square foot                                  | kilogram per square meter                 | 4.882 43                       |
| Pound (force)                                          | kilogram (force)                          | 0.453 592                      |
|                                                        | newton                                    | 4.448 222                      |
|                                                        | poundal                                   | 32.1740                        |
| Pound per square inch                                  | atmosphere                                | 0.068 046 0                    |
|                                                        | bar                                       | 0.068 948 0                    |
|                                                        | inch of mercury (0°C)                     | 2.036 02                       |
|                                                        | millimeter of mercury (0°C)               | 51.7149                        |
|                                                        | millimeter of water (4°C)                 | 703.070                        |
|                                                        | pascal                                    | 6894.757                       |
|                                                        | pound per square foot                     | 144                            |
| Pound-second per square inch                           | pascal-second                             | 6894.76                        |
| Poundal                                                | gram (force)                              | 14.0981                        |
|                                                        | newton                                    | 0.138 255                      |
|                                                        | pound (force)                             | 0.031 081 0                    |
| Poundal per square foot                                | pascal                                    | 1.488 164                      |
| Poundal-foot                                           | newton-meter                              | 0.042 140 1                    |
| Poundal-second per square foot                         | pascal-second                             | 1.488 164                      |
| Proof (U.S.)                                           | percent alcohol by volume*                | 0.5                            |
| Proton mass                                            | atomic mass unit                          | 1.007 28                       |
|                                                        | gram                                      | $1.6726 \times 10^{-24}$       |
| Puncheon (British)                                     | gallon (British)                          | 70                             |

TABLE 2.7 Conversion Factors (Continued)

| To convert                          | Into                          | Multiply by                 |
|-------------------------------------|-------------------------------|-----------------------------|
| Quad                                | Btu                           | $10^{15}$                   |
|                                     | joule                         | $1.055 \times 10^{18}$      |
| Quadrant                            | circumference*                | 0.25                        |
|                                     | degree (angle)*               | 90                          |
|                                     | gon (grade)*                  | 100                         |
|                                     | minute (angle)*               | 5400                        |
|                                     | radian                        | $(\pi/2)$                   |
| Quadrupole area ( $e\text{ cm}^2$ ) | coulomb meter squared         | $1.602\ 18 \times 10^{-23}$ |
| Quart (British)                     | gallon (British)*             | 0.25                        |
|                                     | liter                         | 1.136 523                   |
|                                     | ounce (British, fluid)*       | 40                          |
|                                     | pint (British)*               | 2                           |
| Quart (U.S., dry)                   | quart (U.S., fluid)           | 1.200 95                    |
|                                     | bushel (U.S.)                 | (1/32)                      |
|                                     | cubic foot                    | 0.038 889 25                |
|                                     | liter                         | 1.101 221                   |
|                                     | peck (U.S.)                   | (1/8)                       |
| Quart (U.S., fluid)                 | pint (U.S., dry)*             | 2                           |
|                                     | gallon (U.S.)*                | 0.25                        |
|                                     | liter                         | 0.946 529                   |
|                                     | ounce (U.S., fluid)*          | 32                          |
|                                     | pint (U.S., fluid)            | 2                           |
| Quartern (British, fluid)           | quart (British)               | 0.832 674                   |
|                                     | gill (British)*               | 0.5                         |
| Quintal (metric)                    | kilogram*                     | 100                         |
| Rad (absorbed dose)                 | gray*                         | 0.01                        |
|                                     | joule per kilogram*           | 0.01                        |
| Radian                              | circumference                 | $(1/2\pi)$                  |
|                                     | degree (angle)                | 57.295 780                  |
|                                     | minute (angle)                | 3437.75                     |
|                                     | quadrant                      | $(2/\pi)$                   |
|                                     | revolution                    | $(1/2\pi)$                  |
| Radian per centimeter               | degree per millimeter         | 5.729 58                    |
|                                     | degree per inch               | 145.531                     |
| Radian per second                   | revolution per minute         | 9.549 30                    |
| Radian per second squared           | revolution per minute squared | 572.958                     |
| Rankin (degree)                     | kelvin                        | (5/9)                       |
| Ream                                | quire*                        | 20                          |
|                                     | sheet                         | 480 or 500                  |
| Register ton                        | cubic foot*                   | 100                         |
|                                     | cubic meter                   | 2.831 685                   |
| Rem (dose equivalent)               | sievert*                      | 0.01                        |
| Revolution                          | degree (angle)                | 360                         |
|                                     | gon*                          | 400                         |
|                                     | quadrant*                     | 4                           |
|                                     | radian                        | $(2\pi)$                    |
| Revolution per minute               | degree (angle) per second*    | 6                           |
|                                     | radian per second             | 0.104 720                   |
| Revolution per minute squared       | radian per second squared     | 0.001 745 33                |
| Revolution per second squared       | radian per second squared     | 6.283 185                   |
|                                     | revolution per minute squared | 3600                        |
| Reyn                                | pascal-second                 | 6894.76                     |
|                                     | pound-second per square inch  | 1                           |

**TABLE 2.7** Conversion Factors (*Continued*)

| To convert               | Into                       | Multiply by                     |
|--------------------------|----------------------------|---------------------------------|
| Rhe                      | per pascal-second*         | 10                              |
| Right angle              | degree*                    | 90                              |
|                          | radian                     | ( $\pi/2$ )                     |
| Rod (British, volume)    | cubic foot*                | 1000                            |
| Rod (surveyer's measure) | chain (Gunter's)*          | 0.25                            |
|                          | foot*                      | 16.5                            |
|                          | link (Gunter's)*           | 25                              |
|                          | meter*                     | 5.0292                          |
| Roentgen                 | coulomb per kilogram       | $2.58 \times 10^{-4}$           |
| Rood (British)           | acre*                      | 0.25                            |
|                          | square meter               | 1011.714 1                      |
| Rydberg                  | joule                      | $2.179\ 87 \times 10^{-18}$     |
| Scruple                  | dram (troy)                | (1/3)                           |
|                          | grain*                     | 20                              |
|                          | gram*                      | 1.295 978 2                     |
|                          | ounce (weight)             | 0.045 714 286                   |
|                          | ounce (troy)               | (1/24)                          |
|                          | pennyweight                | (10/12)                         |
|                          | pound                      | (1/350)                         |
| Second (plane angle)     | degree                     | $2.777\ 78 \times 10^{-4}$      |
|                          | minute                     | (1/60)                          |
|                          | radian                     | ( $\pi/6.48 \times 10^5$ )      |
| Section                  | square mile*               | 1                               |
| Siemens                  | mho ( $\text{ohm}^{-1}$ )* | 1                               |
| Slug                     | geepound*                  | 1                               |
|                          | kilogram                   | 14.593 90                       |
|                          | pound                      | 32.1740                         |
| Speed of light           | centimeter per second      | $2.997\ 924\ 58 \times 10^{10}$ |
| Sphere                   | steradian                  | ( $4\pi$ )                      |
| Square centimeter        | circular mil               | $1.973\ 53 \times 10^5$         |
|                          | circular millimeter        | 127.3240                        |
|                          | square inch                | 0.155 000 31                    |
| Square chain (Gunter's)  | acre*                      | 0.1                             |
|                          | square foot*               | 4356                            |
|                          | square meter               | 404.686                         |
| Square chain (Ramsden's) | square foot*               | $10^4$                          |
| Square degree (angle)    | steradian                  | $3.046\ 17 \times 10^{-4}$      |
| Square foot              | acre                       | $2.295\ 68 \times 10^{-5}$      |
|                          | square centimeter          | 929.0304                        |
|                          | square meter               | 0.092 903 04                    |
|                          | square rod                 | 0.003 673 09                    |
| Square inch              | circular mil               | $1.273\ 240 \times 10^6$        |
|                          | circular millimeter        | 821.4432                        |
|                          | square centimeter          | 6.4516                          |
| Square kilometer         | acre                       | 247.1054                        |
|                          | hectare*                   | 100                             |
|                          | square mile                | 0.386 102 16                    |
| Square link (Gunter's)   | square foot*               | 0.4356                          |
| Square link (Ramsden's)  | square foot*               | 1                               |
| Square meter             | are*                       | 0.01                            |
|                          | square foot                | 10.763 91                       |
|                          | square mile                | $3.861\ 01 \times 10^{-7}$      |

TABLE 2.7 Conversion Factors (Continued)

| To convert                        | Into                          | Multiply by                  |
|-----------------------------------|-------------------------------|------------------------------|
| Square meter ( <i>continued</i> ) | square rod                    | 0.039 536 9                  |
|                                   | square yard                   | 1.195 990                    |
| Square mile                       | acre*                         | 640                          |
|                                   | square kilometer              | 2.589 988 110                |
| Square rod                        | township                      | (1/36)                       |
|                                   | acre                          | (1/160)                      |
|                                   | square foot                   | 272.25                       |
|                                   | square meter                  | 25.292 853                   |
| Square yard                       | square foot*                  | 9                            |
|                                   | square inch*                  | 1296                         |
|                                   | square meter*                 | 0.836 127 36                 |
|                                   | square rod                    | 0.033 057 85                 |
| Statampere                        | ampere                        | $3.335\ 641 \times 10^{-10}$ |
| Statcoulomb                       | coulomb                       | $3.335\ 641 \times 10^{-10}$ |
| Statfarad                         | farad                         | $1.112\ 650 \times 10^{-12}$ |
| Stathenry                         | henry                         | $8.987\ 552 \times 10^{11}$  |
| Statmho                           | siemens                       | $1.112\ 650 \times 10^{-12}$ |
| Statohm                           | ohm                           | $8.987\ 552 \times 10^{11}$  |
| Statvolt                          | volt                          | 299.7925                     |
| Statweber                         | weber                         | 299.7925                     |
| Steradian                         | sphere                        | (1/4 $\pi$ )                 |
|                                   | spherical right angle         | (2/ $\pi$ )                  |
|                                   | square degree                 | 3282.81                      |
| Stere                             | cubic meter*                  | 1                            |
| Stilb                             | candela/cm <sup>2</sup>       | 1                            |
| Stokes (kinematic viscosity)      | square meter per second*      | 10 <sup>-4</sup>             |
| Stone (British)                   | pound*                        | 14                           |
| Svedberg                          | second*                       | 10 <sup>-13</sup>            |
| Tablespoon (metric)               | cubic centimeter*; milliter   | 14.79                        |
| Teaspoon (metric)                 | cubic centimeter*; milliliter | 4.929                        |
| Tesla                             | weber per square meter*       | 1                            |
| Tex                               | denier*                       | 9                            |
|                                   | gram per kilometer*           | 1                            |
| Therm                             | Btu*                          | 10 <sup>5</sup>              |
|                                   | joule*                        | $1.054\ 804 \times 10^8$     |
| Ton (assay)                       | gram                          | 29.166 67                    |
| Ton (long)                        | hundredweight (long)*         | 20                           |
|                                   | hundredweight (short)*        | 22.4                         |
|                                   | kilogram                      | 1016.046 908 8               |
|                                   | pound*                        | 2240                         |
|                                   | ton (metric)                  | 1.016 046 9                  |
| Ton (metric)                      | ton (short)                   | 1.12                         |
|                                   | hundredweight (long)          | 19.684 131                   |
|                                   | hundredweight (short)         | 22.046 226                   |
|                                   | kilogram*                     | 1000                         |
|                                   | pound                         | 2204.6226                    |
| Ton (short)                       | ton (long)                    | 0.984 206 53                 |
|                                   | ton (short)*                  | 1.102 311 3                  |
|                                   | kilogram                      | 907.184 74                   |
| Ton (force, long)                 | pound*                        | 2000                         |
|                                   | newton                        | 1186.553                     |
| Ton (force, metric)               | newton                        | 9806.65                      |

**TABLE 2.7** Conversion Factors (*Continued*)

| To convert                         | Into                         | Multiply by                  |
|------------------------------------|------------------------------|------------------------------|
| Ton (force, short)                 | newton                       | 8896.44                      |
| Ton (force, long)/ft <sup>2</sup>  | bar                          | 1.072 518                    |
|                                    | pascal                       | 1.072 518 × 10 <sup>5</sup>  |
| Ton (force, metric)/m <sup>2</sup> | bar                          | 0.098 066 5                  |
|                                    | pascal                       | 9806.65                      |
| Ton (force, short)/ft <sup>2</sup> | bar                          | 0.957 605                    |
|                                    | pascal                       | 9.576 05 × 10 <sup>4</sup>   |
| Tonne (metric)                     | kilogram*                    | 1000                         |
| Torr                               | atmosphere                   | (1/760)                      |
|                                    | millibar                     | 1.333 224                    |
|                                    | millimeter of mercury* (0°C) | 1                            |
|                                    | pascal                       | 133.322; (101 325/760)       |
| Township (U.S.)                    | square kilometer             | 93.2396                      |
|                                    | square mile*                 | 36                           |
| Unified atomic mass unit           | kilogram                     | 1.660 54 × 10 <sup>-27</sup> |
| Unit pole                          | weber                        | 1.256 637 × 10 <sup>-7</sup> |
| Volt (mean international)          | volt                         | 1.000 34                     |
| Volt (U.S. international)          | volt                         | 1.000 330                    |
| Volt-second                        | weber*                       | 1                            |
| Watt                               | Btu per hour                 | 3.412 14                     |
|                                    | calorie per minute           | 14.3308                      |
|                                    | erg per second*              | 10 <sup>7</sup>              |
|                                    | foot-pound per minute        | 44.2537                      |
|                                    | horsepower (British)         | 0.001 341 02                 |
|                                    | horsepower (metric)          | 0.001 359 62                 |
|                                    | joule per second*            | 1                            |
|                                    | kilogram-meter per second    | 0.101 972                    |
| Watt per square inch               | watt per square meter        | 1550.003                     |
| Watt-hour                          | Btu                          | 3.412 14                     |
|                                    | calorie                      | 859.845                      |
|                                    | foot-pound                   | 2655.22                      |
|                                    | horsepower-hour (British)    | 0.001 341 02                 |
|                                    | horsepower-hour (metric)     | 0.001 359 62                 |
|                                    | joule*                       | 3600                         |
|                                    | liter-atmosphere             | 35.5292                      |
| Watt-second                        | joule*                       | 1                            |
| Weber                              | maxwell*                     | 10 <sup>8</sup>              |
| Week                               | day*                         | 7                            |
|                                    | hour*                        | 168                          |
| Wey (British, capacity)            | bushel (British)             | 40 (variable)                |
| Wey (British, mass)                | pound                        | 252 (variable)               |
| X unit                             | meter                        | 1.002 02 × 10 <sup>-13</sup> |
| Yard                               | fathom*                      | 0.5                          |
|                                    | meter                        | 0.9144                       |
| Year (mean of 4-years)             | day                          | 365.25                       |
|                                    | week                         | 52.178 87                    |
| Year (sidereal)                    | day (mean solar)             | 365.256 36                   |

**TABLE 2.8** Temperature Conversion Table

The column of figures in bold and which is headed “Reading in °F. or °C. to be converted” refers to the temperature either in degrees Fahrenheit or Celsius which it is desired to convert into the other scale. If converting from Fahrenheit degrees to Celsius degrees, the equivalent temperature will be found in the column headed “°C.”; while if converting from degrees Celsius to degrees Fahrenheit, the equivalent temperature will be found in the column headed “°F.” This arrangement is very similar to that of Sauveur and Boylston, copyrighted 1920, and is published with their permission.

| °F.   | Reading in<br>°F. or °C.<br>to be<br>converted | °C.     | °F.   | Reading in<br>°F. or °C.<br>to be<br>converted | °C.     |
|-------|------------------------------------------------|---------|-------|------------------------------------------------|---------|
| ..... | —458                                           | —272.22 | ..... | —378                                           | —227.78 |
| ..... | —456                                           | —271.11 | ..... | —376                                           | —226.67 |
| ..... | —454                                           | —270.00 | ..... | —374                                           | —225.56 |
| ..... | —452                                           | —268.89 | ..... | —372                                           | —224.44 |
| ..... | —450                                           | —267.78 | ..... | —370                                           | —223.33 |
| ..... | —448                                           | —266.67 | ..... | —368                                           | —222.22 |
| ..... | —446                                           | —265.56 | ..... | —366                                           | —221.11 |
| ..... | —444                                           | —264.44 | ..... | —364                                           | —220.00 |
| ..... | —442                                           | —263.33 | ..... | —362                                           | —218.89 |
| ..... | —440                                           | —262.22 | ..... | —360                                           | —217.78 |
| ..... | —438                                           | —261.11 | ..... | —358                                           | —216.67 |
| ..... | —436                                           | —260.00 | ..... | —356                                           | —215.56 |
| ..... | —434                                           | —258.89 | ..... | —354                                           | —214.44 |
| ..... | —432                                           | —257.78 | ..... | —352                                           | —213.33 |
| ..... | —430                                           | —256.67 | ..... | —350                                           | —212.22 |
| ..... | —428                                           | —255.56 | ..... | —348                                           | —211.11 |
| ..... | —426                                           | —254.44 | ..... | —346                                           | —210.00 |
| ..... | —424                                           | —253.33 | ..... | —344                                           | —208.89 |
| ..... | —422                                           | —252.22 | ..... | —342                                           | —207.78 |
| ..... | —420                                           | —251.11 | ..... | —340                                           | —206.67 |
| ..... | —418                                           | —250.00 | ..... | —338                                           | —205.56 |
| ..... | —416                                           | —248.89 | ..... | —336                                           | —204.44 |
| ..... | —414                                           | —247.78 | ..... | —334                                           | —203.33 |
| ..... | —412                                           | —246.67 | ..... | —332                                           | —202.22 |
| ..... | —410                                           | —245.56 | ..... | —330                                           | —201.11 |
| ..... | —408                                           | —244.44 | ..... | —328                                           | —200.00 |
| ..... | —406                                           | —243.33 | ..... | —326                                           | —198.89 |
| ..... | —404                                           | —242.22 | ..... | —324                                           | —197.78 |
| ..... | —402                                           | —241.11 | ..... | —322                                           | —196.67 |
| ..... | —400                                           | —240.00 | ..... | —320                                           | —195.56 |
| ..... | —398                                           | —238.89 | ..... | —318                                           | —194.44 |
| ..... | —396                                           | —237.78 | ..... | —316                                           | —193.33 |
| ..... | —394                                           | —236.67 | ..... | —314                                           | —192.22 |
| ..... | —392                                           | —235.56 | ..... | —312                                           | —191.11 |
| ..... | —390                                           | —234.44 | ..... | —310                                           | —190.00 |
| ..... | —388                                           | —233.33 | ..... | —308                                           | —188.89 |
| ..... | —386                                           | —232.22 | ..... | —306                                           | —187.78 |
| ..... | —384                                           | —231.11 | ..... | —304                                           | —186.67 |
| ..... | —382                                           | —230.00 | ..... | —302                                           | —185.56 |
| ..... | —380                                           | —228.89 | ..... | —300                                           | —184.44 |

**TABLE 2.8** Temperature Conversion Table (*Continued*)

| Reading in<br>°F. or °C.<br>to be<br>converted |      |         | Reading in<br>°F. or °C.<br>to be<br>converted |      |         |
|------------------------------------------------|------|---------|------------------------------------------------|------|---------|
| °F.                                            |      | °C.     | °F.                                            |      | °C.     |
| .....                                          | −298 | −183.33 | −342.4                                         | −208 | −133.33 |
| .....                                          | −296 | −182.22 | −338.8                                         | −206 | −132.22 |
| .....                                          | −294 | −181.11 | −335.2                                         | −204 | −131.11 |
| .....                                          | −292 | −180.00 | −331.6                                         | −202 | −130.00 |
| .....                                          | −290 | −178.89 | −328.0                                         | −200 | −128.89 |
| .....                                          | −288 | −177.78 | −324.4                                         | −198 | −127.78 |
| .....                                          | −286 | −176.67 | −320.8                                         | −196 | −126.67 |
| .....                                          | −284 | −175.56 | −317.2                                         | −194 | −125.56 |
| .....                                          | −282 | −174.44 | −313.6                                         | −192 | −124.44 |
| .....                                          | −280 | −173.33 | −310.0                                         | −190 | −123.33 |
| .....                                          | −278 | −172.22 | −306.4                                         | −188 | −122.22 |
| .....                                          | −276 | −171.11 | −302.8                                         | −186 | −121.11 |
| .....                                          | −274 | −170.00 | −299.2                                         | −184 | −120.00 |
| −457.6                                         | −272 | −168.89 | −295.6                                         | −182 | −118.89 |
| −454.0                                         | −270 | −167.78 | −292.0                                         | −180 | −117.78 |
| −450.4                                         | −268 | −166.67 | −288.4                                         | −178 | −116.67 |
| −446.8                                         | −266 | −165.56 | −284.8                                         | −176 | −115.56 |
| −443.2                                         | −264 | −164.44 | −281.2                                         | −174 | −114.44 |
| −439.6                                         | −262 | −163.33 | −277.6                                         | −172 | −113.33 |
| −436.0                                         | −260 | −162.22 | −274.0                                         | −170 | −112.22 |
| −432.4                                         | −258 | −161.11 | −270.4                                         | −168 | −111.11 |
| −428.8                                         | −256 | −160.00 | −266.8                                         | −166 | −110.00 |
| −425.2                                         | −254 | −158.89 | −263.2                                         | −164 | −108.89 |
| −421.6                                         | −252 | −157.78 | −259.6                                         | −162 | −107.78 |
| −418.0                                         | −250 | −156.67 | −256.0                                         | −160 | −106.67 |
| −414.4                                         | −248 | −155.56 | −252.4                                         | −158 | −105.56 |
| −410.8                                         | −246 | −154.44 | −248.8                                         | −156 | −104.44 |
| −407.2                                         | −244 | −153.33 | −245.2                                         | −154 | −103.33 |
| −403.6                                         | −242 | −152.22 | −241.6                                         | −152 | −102.22 |
| −400.0                                         | −240 | −151.11 | −238.0                                         | −150 | −101.11 |
| −396.4                                         | −238 | −150.00 | −234.4                                         | −148 | −100.00 |
| −392.8                                         | −236 | −148.89 | −230.8                                         | −146 | −98.89  |
| −389.2                                         | −234 | −147.78 | −227.2                                         | −144 | −97.78  |
| −385.6                                         | −232 | −146.67 | −223.6                                         | −142 | −96.67  |
| −382.0                                         | −230 | −145.56 | −220.0                                         | −140 | −95.56  |
| −378.4                                         | −228 | −144.44 | −216.4                                         | −138 | −94.44  |
| −374.8                                         | −226 | −143.33 | −212.8                                         | −136 | −93.33  |
| −371.2                                         | −224 | −142.22 | −209.2                                         | −134 | −92.22  |
| −367.6                                         | −222 | −141.11 | −205.6                                         | −132 | −91.11  |
| −364.0                                         | −220 | −140.00 | −202.0                                         | −130 | −90.00  |
| −360.4                                         | −218 | −138.89 | −198.4                                         | −128 | −88.89  |
| −356.8                                         | −216 | −137.78 | −194.8                                         | −126 | −87.78  |
| −353.2                                         | −214 | −136.67 | −191.2                                         | −124 | −86.67  |
| −349.6                                         | −212 | −135.56 | −187.6                                         | −122 | −85.56  |
| −346.0                                         | −210 | −134.44 | −184.0                                         | −120 | −84.44  |

TABLE 2.8 Temperature Conversion Table (Continued)

| Reading in<br>°F. or °C.<br>to be<br>converted |      |        | Reading in<br>°F. or °C.<br>to be<br>converted |     |        |
|------------------------------------------------|------|--------|------------------------------------------------|-----|--------|
| °F.                                            |      | °C.    | °F.                                            |     | °C.    |
| −180.4                                         | −118 | −83.33 | −18.4                                          | −28 | −33.33 |
| −176.8                                         | −116 | −82.22 | −14.8                                          | −26 | −32.22 |
| −173.2                                         | −114 | −81.11 | −11.2                                          | −24 | −31.11 |
| −169.6                                         | −112 | −80.00 | −7.6                                           | −22 | −30.00 |
| −166.0                                         | −110 | −78.89 | −4.0                                           | −20 | −28.89 |
| −162.4                                         | −108 | −77.78 | −0.4                                           | −18 | −27.78 |
| −158.8                                         | −106 | −76.67 | +3.2                                           | −16 | −26.67 |
| −155.2                                         | −104 | −75.56 | +6.8                                           | −14 | −25.56 |
| −151.6                                         | −102 | −74.44 | +10.4                                          | −12 | −24.44 |
| −148.0                                         | −100 | −73.33 | +14.0                                          | −10 | −23.33 |
| −144.4                                         | −98  | −72.22 | +17.6                                          | −8  | −22.22 |
| −140.8                                         | −96  | −71.11 | +19.4                                          | −7  | −21.67 |
| −137.2                                         | −94  | −70.00 | +21.2                                          | −6  | −21.11 |
| −133.6                                         | −92  | −68.89 | +23.0                                          | −5  | −20.56 |
| −130.0                                         | −90  | −67.78 | +24.8                                          | −4  | −20.00 |
| −126.4                                         | −88  | −66.67 | +26.6                                          | −3  | −19.44 |
| −122.8                                         | −86  | −65.56 | +28.4                                          | −2  | −18.89 |
| −119.2                                         | −84  | −64.44 | +30.2                                          | −1  | −18.33 |
| −115.6                                         | −82  | −63.33 | +32.0                                          | ±0  | −17.78 |
| −112.0                                         | −80  | −62.22 | +33.8                                          | +1  | −17.22 |
| −108.4                                         | −78  | −61.11 | +35.6                                          | +2  | −16.67 |
| −104.8                                         | −76  | −60.00 | +37.4                                          | +3  | −16.11 |
| −101.2                                         | −74  | −58.89 | +39.2                                          | +4  | −15.56 |
| −97.6                                          | −72  | −57.78 | +41.0                                          | +5  | −15.00 |
| −94.0                                          | −70  | −56.67 | +42.8                                          | +6  | −14.44 |
| −90.4                                          | −68  | −55.56 | +44.6                                          | +7  | −13.89 |
| −86.8                                          | −66  | −54.44 | +46.4                                          | +8  | −13.33 |
| −83.2                                          | −64  | −53.33 | +48.2                                          | +9  | −12.78 |
| −79.6                                          | −62  | −52.22 | +50.0                                          | +10 | −12.22 |
| −76.0                                          | −60  | −51.11 | +51.8                                          | +11 | −11.67 |
| −72.4                                          | −58  | −50.00 | +53.6                                          | +12 | −11.11 |
| −68.8                                          | −56  | −48.89 | +55.4                                          | +13 | −10.56 |
| −65.2                                          | −54  | −47.78 | +57.2                                          | +14 | −10.00 |
| −61.6                                          | −52  | −46.67 | +59.0                                          | +15 | −9.44  |
| −58.0                                          | −50  | −45.56 | +60.8                                          | +16 | −8.89  |
| −54.4                                          | −48  | −44.44 | +62.6                                          | +17 | −8.33  |
| −50.8                                          | −46  | −43.33 | +64.4                                          | +18 | −7.78  |
| −47.2                                          | −44  | −42.22 | +66.2                                          | +19 | −7.22  |
| −43.6                                          | −42  | −41.11 | +68.0                                          | +20 | −6.67  |
| −40.0                                          | −40  | −40.00 | +69.8                                          | +21 | −6.11  |
| −36.4                                          | −38  | −38.89 | +71.6                                          | +22 | −5.56  |
| −32.8                                          | −36  | −37.78 | +73.4                                          | +23 | −5.00  |
| −29.2                                          | −34  | −36.67 | +75.2                                          | +24 | −4.44  |
| −25.6                                          | −32  | −35.56 | +77.0                                          | +25 | −3.89  |
| −22.0                                          | −30  | −34.44 | +78.8                                          | +26 | −3.33  |



**TABLE 2.8** Temperature Conversion Table (*Continued*)

| Reading in<br>°F. or °C.<br>to be<br>converted |      |         | Reading in<br>°F. or °C.<br>to be<br>converted |       |         |
|------------------------------------------------|------|---------|------------------------------------------------|-------|---------|
| °F.                                            |      | °C.     | °F.                                            |       | °C.     |
| + 80.6                                         | + 27 | − 2.78  | + 161.6                                        | + 72  | + 22.22 |
| + 82.4                                         | + 28 | − 2.22  | + 163.4                                        | + 73  | + 22.78 |
| + 84.2                                         | + 29 | − 1.67  | + 165.2                                        | + 74  | + 23.33 |
| + 86.0                                         | + 30 | − 1.11  | + 167.0                                        | + 75  | + 23.89 |
| + 87.8                                         | + 31 | − 0.56  | + 168.8                                        | + 76  | + 24.44 |
| + 89.6                                         | + 32 | ± 0.00  | + 170.6                                        | + 77  | + 25.00 |
| + 91.4                                         | + 33 | + 0.56  | + 172.4                                        | + 78  | + 25.56 |
| + 93.2                                         | + 34 | + 1.11  | + 174.2                                        | + 79  | + 26.11 |
| + 95.0                                         | + 35 | + 1.67  | + 176.0                                        | + 80  | + 26.67 |
| + 96.8                                         | + 36 | + 2.22  | + 177.8                                        | + 81  | + 27.22 |
| + 98.6                                         | + 37 | + 2.78  | + 179.6                                        | + 82  | + 27.78 |
| + 100.4                                        | + 38 | + 3.33  | + 181.4                                        | + 83  | + 28.33 |
| + 102.2                                        | + 39 | + 3.89  | + 183.2                                        | + 84  | + 28.89 |
| + 104.0                                        | + 40 | + 4.44  | + 185.0                                        | + 85  | + 29.44 |
| + 105.8                                        | + 41 | + 5.00  | + 186.8                                        | + 86  | + 30.00 |
| + 107.6                                        | + 42 | + 5.56  | + 188.6                                        | + 87  | + 30.56 |
| + 109.4                                        | + 43 | + 6.11  | + 190.4                                        | + 88  | + 31.11 |
| + 111.2                                        | + 44 | + 6.67  | + 192.2                                        | + 89  | + 31.67 |
| + 113.0                                        | + 45 | + 7.22  | + 194.0                                        | + 90  | + 32.22 |
| + 114.8                                        | + 46 | + 7.78  | + 195.8                                        | + 91  | + 32.78 |
| + 116.6                                        | + 47 | + 8.33  | + 197.6                                        | + 92  | + 33.33 |
| + 118.4                                        | + 48 | + 8.89  | + 199.4                                        | + 93  | + 33.89 |
| + 120.2                                        | + 49 | + 9.44  | + 201.2                                        | + 94  | + 34.44 |
| + 122.0                                        | + 50 | + 10.00 | + 203.0                                        | + 95  | + 35.00 |
| + 123.8                                        | + 51 | + 10.56 | + 204.8                                        | + 96  | + 35.56 |
| + 125.6                                        | + 52 | + 11.11 | + 206.6                                        | + 97  | + 36.11 |
| + 127.4                                        | + 53 | + 11.67 | + 208.4                                        | + 98  | + 36.67 |
| + 129.2                                        | + 54 | + 12.22 | + 210.2                                        | + 99  | + 37.22 |
| + 131.0                                        | + 55 | + 12.78 | + 212.0                                        | + 100 | + 37.78 |
| + 132.8                                        | + 56 | + 13.33 | + 213.8                                        | + 101 | + 38.33 |
| + 134.6                                        | + 57 | + 13.89 | + 215.6                                        | + 102 | + 38.89 |
| + 136.4                                        | + 58 | + 14.44 | + 217.4                                        | + 103 | + 39.44 |
| + 138.2                                        | + 59 | + 15.00 | + 219.2                                        | + 104 | + 40.00 |
| + 140.0                                        | + 60 | + 15.56 | + 221.0                                        | + 105 | + 40.56 |
| + 141.8                                        | + 61 | + 16.11 | + 222.8                                        | + 106 | + 41.11 |
| + 143.6                                        | + 62 | + 16.67 | + 224.6                                        | + 107 | + 41.67 |
| + 145.4                                        | + 63 | + 17.22 | + 226.4                                        | + 108 | + 42.22 |
| + 147.2                                        | + 64 | + 17.78 | + 228.2                                        | + 109 | + 42.78 |
| + 149.0                                        | + 65 | + 18.33 | + 230.0                                        | + 110 | + 43.33 |
| + 150.8                                        | + 66 | + 18.89 | + 231.8                                        | + 111 | + 43.89 |
| + 152.6                                        | + 67 | + 19.44 | + 233.6                                        | + 112 | + 44.44 |
| + 154.4                                        | + 68 | + 20.00 | + 235.4                                        | + 113 | + 45.00 |
| + 156.2                                        | + 69 | + 20.56 | + 237.2                                        | + 114 | + 45.56 |
| + 158.0                                        | + 70 | + 21.11 | + 239.0                                        | + 115 | + 46.11 |
| + 159.8                                        | + 71 | + 21.67 | + 240.8                                        | + 116 | + 46.67 |

TABLE 2.8    Temperature Conversion Table (*Continued*)

| Reading in<br>°F. or °C.<br>to be<br>converted |       |         | Reading in<br>°F. or °C.<br>to be<br>converted |       |         |
|------------------------------------------------|-------|---------|------------------------------------------------|-------|---------|
| °F.                                            |       | °C.     | °F.                                            |       | °C.     |
| + 242.6                                        | + 117 | + 47.22 | + 323.6                                        | + 162 | + 72.22 |
| + 244.4                                        | + 118 | + 47.78 | + 325.4                                        | + 163 | + 72.78 |
| + 246.2                                        | + 119 | + 48.33 | + 327.2                                        | + 164 | + 73.33 |
| + 248.0                                        | + 120 | + 48.89 | + 329.0                                        | + 165 | + 73.89 |
| + 249.8                                        | + 121 | + 49.44 | + 330.8                                        | + 166 | + 74.44 |
| + 251.6                                        | + 122 | + 50.00 | + 332.6                                        | + 167 | + 75.00 |
| + 253.4                                        | + 123 | + 50.56 | + 334.4                                        | + 168 | + 75.56 |
| + 255.2                                        | + 124 | + 51.11 | + 336.2                                        | + 169 | + 76.11 |
| + 257.0                                        | + 125 | + 51.67 | + 338.0                                        | + 170 | + 76.67 |
| + 258.8                                        | + 126 | + 52.22 | + 339.8                                        | + 171 | + 77.22 |
| + 260.6                                        | + 127 | + 52.78 | + 341.6                                        | + 172 | + 77.78 |
| + 262.4                                        | + 128 | + 53.33 | + 343.4                                        | + 173 | + 78.33 |
| + 264.2                                        | + 129 | + 53.89 | + 345.2                                        | + 174 | + 78.89 |
| + 266.0                                        | + 130 | + 54.44 | + 347.0                                        | + 175 | + 79.44 |
| + 267.8                                        | + 131 | + 55.00 | + 348.8                                        | + 176 | + 80.00 |
| + 269.6                                        | + 132 | + 55.56 | + 350.6                                        | + 177 | + 80.56 |
| + 271.4                                        | + 133 | + 56.11 | + 352.4                                        | + 178 | + 81.11 |
| + 273.2                                        | + 134 | + 56.67 | + 354.2                                        | + 179 | + 81.67 |
| + 275.0                                        | + 135 | + 57.22 | + 356.0                                        | + 180 | + 82.22 |
| + 276.8                                        | + 136 | + 57.78 | + 357.8                                        | + 181 | + 82.78 |
| + 278.6                                        | + 137 | + 58.33 | + 359.6                                        | + 182 | + 83.33 |
| + 280.4                                        | + 138 | + 58.89 | + 361.4                                        | + 183 | + 83.89 |
| + 282.2                                        | + 139 | + 59.44 | + 363.2                                        | + 184 | + 84.44 |
| + 284.0                                        | + 140 | + 60.00 | + 365.0                                        | + 185 | + 85.00 |
| + 285.8                                        | + 141 | + 60.56 | + 366.8                                        | + 186 | + 85.56 |
| + 287.6                                        | + 142 | + 61.11 | + 368.6                                        | + 187 | + 86.11 |
| + 289.4                                        | + 143 | + 61.67 | + 370.4                                        | + 188 | + 86.67 |
| + 291.2                                        | + 144 | + 62.22 | + 372.2                                        | + 189 | + 87.22 |
| + 293.0                                        | + 145 | + 62.78 | + 374.0                                        | + 190 | + 87.78 |
| + 294.8                                        | + 146 | + 63.33 | + 375.8                                        | + 191 | + 88.33 |
| + 296.6                                        | + 147 | + 63.89 | + 377.6                                        | + 192 | + 88.89 |
| + 298.4                                        | + 148 | + 64.44 | + 379.4                                        | + 193 | + 89.44 |
| + 300.2                                        | + 149 | + 65.00 | + 381.2                                        | + 194 | + 90.00 |
| + 302.0                                        | + 150 | + 65.56 | + 383.0                                        | + 195 | + 90.56 |
| + 303.8                                        | + 151 | + 66.11 | + 384.8                                        | + 196 | + 91.11 |
| + 305.6                                        | + 152 | + 66.67 | + 386.6                                        | + 197 | + 91.67 |
| + 307.4                                        | + 153 | + 67.22 | + 388.4                                        | + 198 | + 92.22 |
| + 309.2                                        | + 154 | + 67.78 | + 390.2                                        | + 199 | + 92.78 |
| + 311.0                                        | + 155 | + 68.33 | + 392.0                                        | + 200 | + 93.33 |
| + 312.8                                        | + 156 | + 68.89 | + 393.8                                        | + 201 | + 93.89 |
| + 314.6                                        | + 157 | + 69.44 | + 395.6                                        | + 202 | + 94.44 |
| + 316.4                                        | + 158 | + 70.00 | + 397.4                                        | + 203 | + 95.00 |
| + 318.2                                        | + 159 | + 70.56 | + 399.2                                        | + 204 | + 95.56 |
| + 320.0                                        | + 160 | + 71.11 | + 401.0                                        | + 205 | + 96.11 |
| + 321.8                                        | + 161 | + 71.67 | + 402.8                                        | + 206 | + 96.67 |

**TABLE 2.8** Temperature Conversion Table (*Continued*)

| °F.     | Reading in<br>°F. or °C.<br>to be<br>converted | °C.      | °F.     | Reading in<br>°F. or °C.<br>to be<br>converted | °C.      |
|---------|------------------------------------------------|----------|---------|------------------------------------------------|----------|
| + 404.6 | + 207                                          | + 97.22  | + 543.2 | + 284                                          | + 140.00 |
| + 406.4 | + 208                                          | + 97.78  | + 546.8 | + 286                                          | + 141.11 |
| + 408.2 | + 209                                          | + 98.33  | + 550.4 | + 288                                          | + 142.22 |
| + 410.0 | + 210                                          | + 98.89  | + 554.0 | + 290                                          | + 143.33 |
| + 411.8 | + 211                                          | + 99.44  | + 557.6 | + 292                                          | + 144.44 |
| + 413.6 | + 212                                          | + 100.00 | + 561.2 | + 294                                          | + 145.56 |
| + 415.4 | + 213                                          | + 100.56 | + 564.8 | + 296                                          | + 146.67 |
| + 417.2 | + 214                                          | + 101.11 | + 568.4 | + 298                                          | + 147.78 |
| + 419.0 | + 215                                          | + 101.67 | + 572.0 | + 300                                          | + 148.89 |
| + 420.8 | + 216                                          | + 102.22 | + 575.6 | + 302                                          | + 150.00 |
| + 422.6 | + 217                                          | + 102.78 | + 579.2 | + 304                                          | + 151.11 |
| + 424.4 | + 218                                          | + 103.33 | + 582.8 | + 306                                          | + 152.22 |
| + 426.2 | + 219                                          | + 103.89 | + 586.4 | + 308                                          | + 153.33 |
| + 428.0 | + 220                                          | + 104.44 | + 590.0 | + 310                                          | + 154.44 |
| + 431.6 | + 222                                          | + 105.56 | + 593.6 | + 312                                          | + 155.56 |
| + 435.2 | + 224                                          | + 106.67 | + 597.2 | + 314                                          | + 156.67 |
| + 438.8 | + 226                                          | + 107.78 | + 600.8 | + 316                                          | + 157.78 |
| + 442.4 | + 228                                          | + 108.89 | + 604.4 | + 318                                          | + 158.89 |
| + 446.0 | + 230                                          | + 110.00 | + 608.0 | + 320                                          | + 160.00 |
| + 449.6 | + 232                                          | + 111.11 | + 611.6 | + 322                                          | + 161.11 |
| + 453.2 | + 234                                          | + 112.22 | + 615.2 | + 324                                          | + 162.22 |
| + 456.8 | + 236                                          | + 113.33 | + 618.8 | + 326                                          | + 163.33 |
| + 460.4 | + 238                                          | + 114.44 | + 622.4 | + 328                                          | + 164.44 |
| + 464.0 | + 240                                          | + 115.56 | + 626.0 | + 330                                          | + 165.56 |
| + 467.6 | + 242                                          | + 116.67 | + 629.6 | + 332                                          | + 166.67 |
| + 471.2 | + 244                                          | + 117.78 | + 633.2 | + 334                                          | + 167.78 |
| + 474.8 | + 246                                          | + 118.89 | + 636.8 | + 336                                          | + 168.89 |
| + 478.4 | + 248                                          | + 120.00 | + 640.4 | + 338                                          | + 170.00 |
| + 482.0 | + 250                                          | + 121.11 | + 644.0 | + 340                                          | + 171.11 |
| + 485.6 | + 252                                          | + 122.22 | + 647.6 | + 342                                          | + 172.22 |
| + 489.2 | + 254                                          | + 123.33 | + 651.2 | + 344                                          | + 173.33 |
| + 492.8 | + 256                                          | + 124.44 | + 654.8 | + 346                                          | + 174.44 |
| + 496.4 | + 258                                          | + 125.56 | + 658.4 | + 348                                          | + 175.56 |
| + 500.0 | + 260                                          | + 126.67 | + 662.0 | + 350                                          | + 176.67 |
| + 503.6 | + 262                                          | + 127.78 | + 665.6 | + 352                                          | + 177.78 |
| + 507.2 | + 264                                          | + 128.89 | + 669.2 | + 354                                          | + 178.89 |
| + 510.8 | + 266                                          | + 130.00 | + 672.8 | + 356                                          | + 180.00 |
| + 514.4 | + 268                                          | + 131.11 | + 676.4 | + 358                                          | + 181.11 |
| + 518.0 | + 270                                          | + 132.22 | + 680.0 | + 360                                          | + 182.22 |
| + 521.6 | + 272                                          | + 133.33 | + 683.6 | + 362                                          | + 183.33 |
| + 525.2 | + 274                                          | + 134.44 | + 687.2 | + 364                                          | + 184.44 |
| + 528.8 | + 276                                          | + 135.56 | + 690.8 | + 366                                          | + 185.56 |
| + 532.4 | + 278                                          | + 136.67 | + 694.4 | + 368                                          | + 186.67 |
| + 536.0 | + 280                                          | + 137.78 | + 698.0 | + 370                                          | + 187.78 |
| + 539.6 | + 282                                          | + 138.89 | + 701.6 | + 372                                          | + 188.89 |

TABLE 2.8 Temperature Conversion Table (Continued)

| Reading in<br>°F. or °C.<br>to be<br>converted |       |          | Reading in<br>°F. or °C.<br>to be<br>converted |       |          |
|------------------------------------------------|-------|----------|------------------------------------------------|-------|----------|
| °F.                                            |       | °C.      | °F.                                            |       | °C.      |
| + 705.2                                        | + 374 | + 190.00 | + 867.2                                        | + 464 | + 240.00 |
| + 708.8                                        | + 376 | + 191.11 | + 870.8                                        | + 466 | + 241.11 |
| + 712.4                                        | + 378 | + 192.22 | + 874.4                                        | + 468 | + 242.22 |
| + 716.0                                        | + 380 | + 193.33 | + 878.0                                        | + 470 | + 243.33 |
| + 719.6                                        | + 382 | + 194.44 | + 881.6                                        | + 472 | + 244.44 |
| + 723.2                                        | + 384 | + 195.56 | + 885.2                                        | + 474 | + 245.56 |
| + 726.8                                        | + 386 | + 196.67 | + 888.8                                        | + 476 | + 246.67 |
| + 730.4                                        | + 388 | + 197.78 | + 892.4                                        | + 478 | + 247.78 |
| + 734.0                                        | + 390 | + 198.89 | + 896.0                                        | + 480 | + 248.89 |
| + 737.6                                        | + 392 | + 200.00 | + 899.6                                        | + 482 | + 250.00 |
| + 741.2                                        | + 394 | + 201.11 | + 903.2                                        | + 484 | + 251.11 |
| + 744.8                                        | + 396 | + 202.22 | + 906.8                                        | + 486 | + 252.22 |
| + 748.4                                        | + 398 | + 203.33 | + 910.4                                        | + 488 | + 253.33 |
| + 752.0                                        | + 400 | + 204.44 | + 914.0                                        | + 490 | + 254.44 |
| + 755.6                                        | + 402 | + 205.56 | + 917.6                                        | + 492 | + 255.56 |
| + 759.2                                        | + 404 | + 206.67 | + 921.2                                        | + 494 | + 256.67 |
| + 762.8                                        | + 406 | + 207.78 | + 924.8                                        | + 496 | + 257.78 |
| + 766.4                                        | + 408 | + 208.89 | + 928.4                                        | + 498 | + 258.89 |
| + 770.0                                        | + 410 | + 210.00 | + 932.0                                        | + 500 | + 260.00 |
| + 773.6                                        | + 412 | + 211.11 | + 935.6                                        | + 502 | + 261.11 |
| + 777.2                                        | + 414 | + 212.22 | + 939.2                                        | + 504 | + 262.22 |
| + 780.8                                        | + 416 | + 213.33 | + 942.8                                        | + 506 | + 263.33 |
| + 784.4                                        | + 418 | + 214.44 | + 946.4                                        | + 508 | + 264.44 |
| + 788.0                                        | + 420 | + 215.56 | + 950.0                                        | + 510 | + 265.56 |
| + 791.6                                        | + 422 | + 216.67 | + 953.6                                        | + 512 | + 266.67 |
| + 795.2                                        | + 424 | + 217.78 | + 957.2                                        | + 514 | + 267.78 |
| + 798.8                                        | + 426 | + 218.89 | + 960.8                                        | + 516 | + 268.89 |
| + 802.4                                        | + 428 | + 220.00 | + 964.4                                        | + 518 | + 270.00 |
| + 806.0                                        | + 430 | + 221.11 | + 968.0                                        | + 520 | + 271.11 |
| + 809.6                                        | + 432 | + 222.22 | + 971.6                                        | + 522 | + 272.22 |
| + 813.2                                        | + 434 | + 223.33 | + 975.2                                        | + 524 | + 273.33 |
| + 816.8                                        | + 436 | + 224.44 | + 978.8                                        | + 526 | + 274.44 |
| + 820.4                                        | + 438 | + 225.56 | + 982.4                                        | + 528 | + 275.56 |
| + 824.0                                        | + 440 | + 226.67 | + 986.0                                        | + 530 | + 276.67 |
| + 827.6                                        | + 442 | + 227.78 | + 989.6                                        | + 532 | + 277.78 |
| + 831.2                                        | + 444 | + 228.89 | + 993.2                                        | + 534 | + 278.89 |
| + 834.8                                        | + 446 | + 230.00 | + 996.8                                        | + 536 | + 280.00 |
| + 838.4                                        | + 448 | + 231.11 | + 1000.4                                       | + 538 | + 281.11 |
| + 842.0                                        | + 450 | + 232.22 | + 1004.0                                       | + 540 | + 282.22 |
| + 845.6                                        | + 452 | + 233.33 | + 1007.6                                       | + 542 | + 283.33 |
| + 849.2                                        | + 454 | + 234.44 | + 1011.2                                       | + 544 | + 284.44 |
| + 852.8                                        | + 456 | + 235.56 | + 1014.8                                       | + 546 | + 285.56 |
| + 856.4                                        | + 458 | + 236.67 | + 1018.4                                       | + 548 | + 286.67 |
| + 860.0                                        | + 460 | + 237.78 | + 1022.0                                       | + 550 | + 287.78 |
| + 863.6                                        | + 462 | + 238.89 | + 1025.6                                       | + 552 | + 288.89 |

TABLE 2.8 Temperature Conversion Table (Continued)

| °F.      | Reading in<br>°F. or °C.<br>to be<br>converted | °C.      | °F.      | Reading in<br>°F. or °C.<br>to be<br>converted | °C.      |
|----------|------------------------------------------------|----------|----------|------------------------------------------------|----------|
| + 1029.2 | + 554                                          | + 290.00 | + 1191.2 | + 644                                          | + 340.00 |
| + 1032.8 | + 556                                          | + 291.11 | + 1194.8 | + 646                                          | + 341.11 |
| + 1036.4 | + 558                                          | + 292.22 | + 1198.4 | + 648                                          | + 342.22 |
| + 1040.0 | + 560                                          | + 293.33 | + 1202.0 | + 650                                          | + 343.33 |
| + 1043.6 | + 562                                          | + 294.44 | + 1205.6 | + 652                                          | + 344.44 |
| + 1047.2 | + 564                                          | + 295.56 | + 1209.2 | + 654                                          | + 345.56 |
| + 1050.8 | + 566                                          | + 296.67 | + 1212.8 | + 656                                          | + 346.67 |
| + 1054.4 | + 568                                          | + 297.78 | + 1216.4 | + 658                                          | + 347.78 |
| + 1058.0 | + 570                                          | + 298.89 | + 1220.0 | + 660                                          | + 348.89 |
| + 1061.6 | + 572                                          | + 300.00 | + 1223.6 | + 662                                          | + 350.00 |
| + 1065.2 | + 574                                          | + 301.11 | + 1227.2 | + 664                                          | + 351.11 |
| + 1068.8 | + 576                                          | + 302.22 | + 1230.8 | + 666                                          | + 352.22 |
| + 1072.4 | + 578                                          | + 303.33 | + 1234.4 | + 668                                          | + 353.33 |
| + 1076.0 | + 580                                          | + 304.44 | + 1238.0 | + 670                                          | + 354.44 |
| + 1079.6 | + 582                                          | + 305.56 | + 1241.6 | + 672                                          | + 355.56 |
| + 1083.2 | + 584                                          | + 306.67 | + 1245.2 | + 674                                          | + 356.67 |
| + 1086.8 | + 586                                          | + 307.78 | + 1248.8 | + 676                                          | + 357.78 |
| + 1090.4 | + 588                                          | + 308.89 | + 1252.4 | + 678                                          | + 358.89 |
| + 1094.0 | + 590                                          | + 310.00 | + 1256.0 | + 680                                          | + 360.00 |
| + 1097.6 | + 592                                          | + 311.11 | + 1259.6 | + 682                                          | + 361.11 |
| + 1101.2 | + 594                                          | + 312.22 | + 1263.2 | + 684                                          | + 362.22 |
| + 1104.8 | + 596                                          | + 313.33 | + 1266.8 | + 686                                          | + 363.33 |
| + 1108.4 | + 598                                          | + 314.44 | + 1270.4 | + 688                                          | + 364.44 |
| + 1112.0 | + 600                                          | + 315.56 | + 1274.0 | + 690                                          | + 365.56 |
| + 1115.6 | + 602                                          | + 316.67 | + 1277.6 | + 692                                          | + 366.67 |
| + 1119.2 | + 604                                          | + 317.78 | + 1281.2 | + 694                                          | + 367.78 |
| + 1122.8 | + 606                                          | + 318.89 | + 1284.8 | + 696                                          | + 368.89 |
| + 1126.4 | + 608                                          | + 320.00 | + 1288.4 | + 698                                          | + 370.00 |
| + 1130.0 | + 610                                          | + 321.11 | + 1292.0 | + 700                                          | + 371.11 |
| + 1133.6 | + 612                                          | + 322.22 | + 1295.6 | + 702                                          | + 372.22 |
| + 1137.2 | + 614                                          | + 323.33 | + 1299.2 | + 704                                          | + 373.33 |
| + 1140.8 | + 616                                          | + 324.44 | + 1302.8 | + 706                                          | + 374.44 |
| + 1144.4 | + 618                                          | + 325.56 | + 1306.4 | + 708                                          | + 375.56 |
| + 1148.0 | + 620                                          | + 326.67 | + 1310.0 | + 710                                          | + 376.67 |
| + 1151.6 | + 622                                          | + 327.78 | + 1313.6 | + 712                                          | + 377.78 |
| + 1155.2 | + 624                                          | + 328.89 | + 1317.2 | + 714                                          | + 378.89 |
| + 1158.8 | + 626                                          | + 330.00 | + 1320.8 | + 716                                          | + 380.00 |
| + 1162.4 | + 628                                          | + 331.11 | + 1324.4 | + 718                                          | + 381.11 |
| + 1166.0 | + 630                                          | + 332.22 | + 1328.0 | + 720                                          | + 382.22 |
| + 1169.6 | + 632                                          | + 333.33 | + 1331.6 | + 722                                          | + 383.33 |
| + 1173.2 | + 634                                          | + 334.44 | + 1335.2 | + 724                                          | + 384.44 |
| + 1176.8 | + 636                                          | + 335.56 | + 1338.8 | + 726                                          | + 385.56 |
| + 1180.4 | + 638                                          | + 336.67 | + 1342.4 | + 728                                          | + 386.67 |
| + 1184.0 | + 640                                          | + 337.78 | + 1346.0 | + 730                                          | + 387.78 |
| + 1187.6 | + 642                                          | + 338.89 | + 1349.6 | + 732                                          | + 388.89 |

TABLE 2.8 Temperature Conversion Table (Continued)

| Reading in<br>°F. or °C.<br>to be<br>converted |       |          | Reading in<br>°F. or °C.<br>to be<br>converted |       |          |
|------------------------------------------------|-------|----------|------------------------------------------------|-------|----------|
| °F.                                            |       | °C.      | °F.                                            |       | °C.      |
| + 1353.2                                       | + 734 | + 390.00 | + 1515.2                                       | + 824 | + 440.00 |
| + 1356.8                                       | + 736 | + 391.11 | + 1518.8                                       | + 826 | + 441.11 |
| + 1360.4                                       | + 738 | + 392.22 | + 1522.4                                       | + 828 | + 442.22 |
| + 1364.0                                       | + 740 | + 393.33 | + 1526.0                                       | + 830 | + 443.33 |
| + 1367.6                                       | + 742 | + 394.44 | + 1529.6                                       | + 832 | + 444.44 |
| + 1371.2                                       | + 744 | + 395.56 | + 1533.2                                       | + 834 | + 445.56 |
| + 1374.8                                       | + 746 | + 396.67 | + 1536.8                                       | + 836 | + 446.67 |
| + 1378.4                                       | + 748 | + 397.78 | + 1540.4                                       | + 838 | + 447.78 |
| + 1382.0                                       | + 750 | + 398.89 | + 1544.0                                       | + 840 | + 448.89 |
| + 1385.6                                       | + 752 | + 400.00 | + 1547.6                                       | + 842 | + 450.00 |
| + 1389.2                                       | + 754 | + 401.11 | + 1551.2                                       | + 844 | + 451.11 |
| + 1392.8                                       | + 756 | + 402.22 | + 1554.8                                       | + 846 | + 452.22 |
| + 1396.4                                       | + 758 | + 403.33 | + 1558.4                                       | + 848 | + 453.33 |
| + 1400.0                                       | + 760 | + 404.44 | + 1562.0                                       | + 850 | + 454.44 |
| + 1403.6                                       | + 762 | + 405.56 | + 1565.6                                       | + 852 | + 455.56 |
| + 1407.2                                       | + 764 | + 406.67 | + 1569.2                                       | + 854 | + 456.67 |
| + 1410.8                                       | + 766 | + 407.78 | + 1572.8                                       | + 856 | + 457.78 |
| + 1414.4                                       | + 768 | + 408.89 | + 1576.4                                       | + 858 | + 458.89 |
| + 1418.0                                       | + 770 | + 410.00 | + 1580.0                                       | + 860 | + 460.00 |
| + 1421.6                                       | + 772 | + 411.11 | + 1583.6                                       | + 862 | + 461.11 |
| + 1425.2                                       | + 774 | + 412.22 | + 1587.2                                       | + 864 | + 462.22 |
| + 1428.8                                       | + 776 | + 413.33 | + 1590.8                                       | + 866 | + 463.33 |
| + 1432.4                                       | + 778 | + 414.44 | + 1594.4                                       | + 868 | + 464.44 |
| + 1436.0                                       | + 780 | + 415.56 | + 1598.0                                       | + 870 | + 465.56 |
| + 1439.6                                       | + 782 | + 416.67 | + 1601.6                                       | + 872 | + 466.67 |
| + 1443.2                                       | + 784 | + 417.78 | + 1605.2                                       | + 874 | + 467.78 |
| + 1446.8                                       | + 786 | + 418.89 | + 1608.8                                       | + 876 | + 468.89 |
| + 1450.4                                       | + 788 | + 420.00 | + 1612.4                                       | + 878 | + 470.00 |
| + 1454.0                                       | + 790 | + 421.11 | + 1616.0                                       | + 880 | + 471.11 |
| + 1457.6                                       | + 792 | + 422.22 | + 1619.6                                       | + 882 | + 472.22 |
| + 1461.2                                       | + 794 | + 423.33 | + 1623.2                                       | + 884 | + 473.33 |
| + 1464.8                                       | + 796 | + 424.44 | + 1626.8                                       | + 886 | + 474.44 |
| + 1468.4                                       | + 798 | + 425.56 | + 1630.4                                       | + 888 | + 475.56 |
| + 1472.0                                       | + 800 | + 426.67 | + 1634.0                                       | + 890 | + 476.67 |
| + 1475.6                                       | + 802 | + 427.78 | + 1637.6                                       | + 892 | + 477.78 |
| + 1479.2                                       | + 804 | + 428.89 | + 1641.2                                       | + 894 | + 478.89 |
| + 1482.8                                       | + 806 | + 430.00 | + 1644.8                                       | + 896 | + 480.00 |
| + 1486.4                                       | + 808 | + 431.11 | + 1648.4                                       | + 898 | + 481.11 |
| + 1490.0                                       | + 810 | + 432.22 | + 1652.0                                       | + 900 | + 482.22 |
| + 1493.6                                       | + 812 | + 433.33 | + 1655.6                                       | + 902 | + 483.33 |
| + 1497.2                                       | + 814 | + 434.44 | + 1659.2                                       | + 904 | + 484.44 |
| + 1500.8                                       | + 816 | + 435.56 | + 1662.8                                       | + 906 | + 485.56 |
| + 1504.4                                       | + 818 | + 436.67 | + 1666.4                                       | + 908 | + 486.67 |
| + 1508.0                                       | + 820 | + 437.78 | + 1670.0                                       | + 910 | + 487.78 |
| + 1511.6                                       | + 822 | + 438.89 | + 1673.6                                       | + 912 | + 488.89 |

**TABLE 2.8** Temperature Conversion Table (*Continued*)

| Reading in<br>°F. or °C.<br>to be<br>converted |        |          | Reading in<br>°F. or °C.<br>to be<br>converted |        |          |
|------------------------------------------------|--------|----------|------------------------------------------------|--------|----------|
| °F.                                            |        | °C.      | °F.                                            |        | °C.      |
| + 1677.2                                       | + 914  | + 490.00 | + 1868.0                                       | + 1020 | + 548.89 |
| + 1680.8                                       | + 916  | + 491.11 | + 1886.0                                       | + 1030 | + 554.44 |
| + 1684.4                                       | + 918  | + 492.22 | + 1904.0                                       | + 1040 | + 560.00 |
| + 1688.0                                       | + 920  | + 493.33 | + 1922.0                                       | + 1050 | + 565.56 |
| + 1691.6                                       | + 922  | + 494.44 | + 1940.0                                       | + 1060 | + 571.11 |
| + 1695.2                                       | + 924  | + 495.56 | + 1958.0                                       | + 1070 | + 576.67 |
| + 1698.8                                       | + 926  | + 496.67 | + 1976.0                                       | + 1080 | + 582.22 |
| + 1702.4                                       | + 928  | + 497.78 | + 1994.0                                       | + 1090 | + 587.78 |
| + 1706.0                                       | + 930  | + 498.89 | + 2012.0                                       | + 1100 | + 593.33 |
| + 1709.6                                       | + 932  | + 500.00 | + 2030.0                                       | + 1110 | + 598.89 |
| + 1713.2                                       | + 934  | + 501.11 | + 2048.0                                       | + 1120 | + 604.44 |
| + 1716.8                                       | + 936  | + 502.22 | + 2066.0                                       | + 1130 | + 610.00 |
| + 1720.4                                       | + 938  | + 503.33 | + 2084.0                                       | + 1140 | + 615.56 |
| + 1724.0                                       | + 940  | + 504.44 | + 2102.0                                       | + 1150 | + 621.11 |
| + 1727.6                                       | + 942  | + 505.56 | + 2120.0                                       | + 1160 | + 626.67 |
| + 1731.2                                       | + 944  | + 506.67 | + 2138.0                                       | + 1170 | + 632.22 |
| + 1734.8                                       | + 946  | + 507.78 | + 2156.0                                       | + 1180 | + 637.78 |
| + 1738.4                                       | + 948  | + 508.89 | + 2174.0                                       | + 1190 | + 643.33 |
| + 1742.0                                       | + 950  | + 510.00 | + 2192.0                                       | + 1200 | + 648.89 |
| + 1745.6                                       | + 952  | + 511.11 | + 2210.0                                       | + 1210 | + 654.44 |
| + 1749.2                                       | + 954  | + 512.22 | + 2228.0                                       | + 1220 | + 660.00 |
| + 1752.8                                       | + 956  | + 513.33 | + 2246.0                                       | + 1230 | + 665.56 |
| + 1756.4                                       | + 958  | + 514.44 | + 2264.0                                       | + 1240 | + 671.11 |
| + 1760.0                                       | + 960  | + 515.56 | + 2282.0                                       | + 1250 | + 676.67 |
| + 1763.6                                       | + 962  | + 516.67 | + 2300.0                                       | + 1260 | + 682.22 |
| + 1767.2                                       | + 964  | + 517.78 | + 2318.0                                       | + 1270 | + 687.78 |
| + 1770.8                                       | + 966  | + 518.89 | + 2336.0                                       | + 1280 | + 693.33 |
| + 1774.4                                       | + 968  | + 520.00 | + 2354.0                                       | + 1290 | + 698.89 |
| + 1778.0                                       | + 970  | + 521.11 | + 2372.0                                       | + 1300 | + 704.44 |
| + 1781.6                                       | + 972  | + 522.22 | + 2390.0                                       | + 1310 | + 710.00 |
| + 1785.2                                       | + 974  | + 523.33 | + 2408.0                                       | + 1320 | + 715.56 |
| + 1788.8                                       | + 976  | + 524.44 | + 2426.0                                       | + 1330 | + 721.11 |
| + 1792.4                                       | + 978  | + 525.56 | + 2444.0                                       | + 1340 | + 726.67 |
| + 1796.0                                       | + 980  | + 526.67 | + 2462.0                                       | + 1350 | + 732.22 |
| + 1799.6                                       | + 982  | + 527.78 | + 2480.0                                       | + 1360 | + 737.78 |
| + 1803.2                                       | + 984  | + 528.89 | + 2498.0                                       | + 1370 | + 743.33 |
| + 1806.8                                       | + 986  | + 530.00 | + 2516.0                                       | + 1380 | + 748.89 |
| + 1810.4                                       | + 988  | + 531.11 | + 2534.0                                       | + 1390 | + 754.44 |
| + 1814.0                                       | + 990  | + 532.22 | + 2552.0                                       | + 1400 | + 760.00 |
| + 1817.6                                       | + 992  | + 533.33 | + 2570.0                                       | + 1410 | + 765.56 |
| + 1821.2                                       | + 994  | + 534.44 | + 2588.0                                       | + 1420 | + 771.11 |
| + 1824.8                                       | + 996  | + 535.56 | + 2606.0                                       | + 1430 | + 776.67 |
| + 1828.4                                       | + 998  | + 536.67 | + 2624.0                                       | + 1440 | + 782.22 |
| + 1832.0                                       | + 1000 | + 537.78 | + 2642.0                                       | + 1450 | + 787.78 |
| + 1850.0                                       | + 1010 | + 543.33 | + 2660.0                                       | + 1460 | + 793.33 |

TABLE 2.8 Temperature Conversion Table (Continued)

| Reading in<br>°F. or °C.<br>to be<br>converted |        |          | Reading in<br>°F. or °C.<br>to be<br>converted |        |          |
|------------------------------------------------|--------|----------|------------------------------------------------|--------|----------|
| °F.                                            |        | °C.      | °F.                                            |        | °C.      |
| + 2678.0                                       | + 1470 | + 798.89 | + 3488.0                                       | + 1920 | + 1048.9 |
| + 2696.0                                       | + 1480 | + 804.44 | + 3506.0                                       | + 1930 | + 1054.4 |
| + 2714.0                                       | + 1490 | + 810.00 | + 3524.0                                       | + 1940 | + 1060.0 |
| + 2732.0                                       | + 1500 | + 815.56 | + 3542.0                                       | + 1950 | + 1065.6 |
| + 2750.0                                       | + 1510 | + 821.11 | + 3560.0                                       | + 1960 | + 1071.1 |
| + 2768.0                                       | + 1520 | + 826.67 | + 3578.0                                       | + 1970 | + 1076.7 |
| + 2786.0                                       | + 1530 | + 832.22 | + 3596.0                                       | + 1980 | + 1082.2 |
| + 2804.0                                       | + 1540 | + 837.78 | + 3614.0                                       | + 1990 | + 1087.8 |
| + 2822.0                                       | + 1550 | + 843.33 | + 3632.0                                       | + 2000 | + 1093.3 |
| + 2840.0                                       | + 1560 | + 848.89 | + 3650.0                                       | + 2010 | + 1098.9 |
| + 2858.0                                       | + 1570 | + 854.44 | + 3668.0                                       | + 2020 | + 1104.4 |
| + 2876.0                                       | + 1580 | + 860.00 | + 3686.0                                       | + 2030 | + 1110.0 |
| + 2894.0                                       | + 1590 | + 865.56 | + 3704.0                                       | + 2040 | + 1115.6 |
| + 2912.0                                       | + 1600 | + 871.11 | + 3722.0                                       | + 2050 | + 1121.1 |
| + 2930.0                                       | + 1610 | + 876.67 | + 3740.0                                       | + 2060 | + 1126.7 |
| + 2948.0                                       | + 1620 | + 882.22 | + 3758.0                                       | + 2070 | + 1132.2 |
| + 2966.0                                       | + 1630 | + 887.78 | + 3776.0                                       | + 2080 | + 1137.8 |
| + 2984.0                                       | + 1640 | + 893.33 | + 3794.0                                       | + 2090 | + 1143.3 |
| + 3002.0                                       | + 1650 | + 898.89 | + 3812.0                                       | + 2100 | + 1148.9 |
| + 3020.0                                       | + 1660 | + 904.44 | + 3830.0                                       | + 2110 | + 1154.4 |
| + 3038.0                                       | + 1670 | + 910.00 | + 3848.0                                       | + 2120 | + 1160.0 |
| + 3056.0                                       | + 1680 | + 915.56 | + 3866.0                                       | + 2130 | + 1165.6 |
| + 3074.0                                       | + 1690 | + 921.11 | + 3884.0                                       | + 2140 | + 1171.1 |
| + 3092.0                                       | + 1700 | + 926.67 | + 3902.0                                       | + 2150 | + 1176.7 |
| + 3110.0                                       | + 1710 | + 932.22 | + 3920.0                                       | + 2160 | + 1182.2 |
| + 3128.0                                       | + 1720 | + 937.78 | + 3938.0                                       | + 2170 | + 1187.8 |
| + 3146.0                                       | + 1730 | + 943.33 | + 3956.0                                       | + 2180 | + 1193.3 |
| + 3164.0                                       | + 1740 | + 948.89 | + 3974.0                                       | + 2190 | + 1198.9 |
| + 3182.0                                       | + 1750 | + 954.44 | + 3992.0                                       | + 2200 | + 1204.4 |
| + 3200.0                                       | + 1760 | + 960.00 | + 4010.0                                       | + 2210 | + 1210.0 |
| + 3218.0                                       | + 1770 | + 965.56 | + 4028.0                                       | + 2220 | + 1215.6 |
| + 3236.0                                       | + 1780 | + 971.11 | + 4046.0                                       | + 2230 | + 1221.1 |
| + 3254.0                                       | + 1790 | + 976.67 | + 4064.0                                       | + 2240 | + 1226.7 |
| + 3272.0                                       | + 1800 | + 982.22 | + 4082.0                                       | + 2250 | + 1232.2 |
| + 3290.0                                       | + 1810 | + 987.78 | + 4100.0                                       | + 2260 | + 1237.8 |
| + 3308.0                                       | + 1820 | + 993.33 | + 4118.0                                       | + 2270 | + 1243.3 |
| + 3326.0                                       | + 1830 | + 998.89 | + 4136.0                                       | + 2280 | + 1248.9 |
| + 3344.0                                       | + 1840 | + 1004.4 | + 4154.0                                       | + 2290 | + 1254.4 |
| + 3362.0                                       | + 1850 | + 1010.0 | + 4172.0                                       | + 2300 | + 1260.0 |
| + 3380.0                                       | + 1860 | + 1015.6 | + 4190.0                                       | + 2310 | + 1265.6 |
| + 3398.0                                       | + 1870 | + 1021.1 | + 4208.0                                       | + 2320 | + 1271.1 |
| + 3416.0                                       | + 1880 | + 1026.7 | + 4226.0                                       | + 2330 | + 1276.7 |
| + 3434.0                                       | + 1890 | + 1032.2 | + 4244.0                                       | + 2340 | + 1282.2 |
| + 3452.0                                       | + 1900 | + 1037.8 | + 4262.0                                       | + 2350 | + 1287.8 |
| + 3470.0                                       | + 1910 | + 1043.3 | + 4280.0                                       | + 2360 | + 1293.3 |



TABLE 2.8 Temperature Conversion Table (Continued)

| °F.      | Reading in<br>°F. or °C.<br>to be<br>converted | °C.      | °F.      | Reading in<br>°F. or °C.<br>to be<br>converted | °C.      |
|----------|------------------------------------------------|----------|----------|------------------------------------------------|----------|
| + 4298.0 | + 2370                                         | + 1298.9 | + 4964.0 | + 2740                                         | + 1504.4 |
| + 4316.0 | + 2380                                         | + 1304.4 | + 4982.0 | + 2750                                         | + 1510.0 |
| + 4334.0 | + 2390                                         | + 1310.0 | + 5000.0 | + 2760                                         | + 1515.6 |
| + 4352.0 | + 2400                                         | + 1315.6 | + 5018.0 | + 2770                                         | + 1521.1 |
| + 4370.0 | + 2410                                         | + 1321.1 | + 5036.0 | + 2780                                         | + 1526.7 |
| + 4388.0 | + 2420                                         | + 1326.7 | + 5054.0 | + 2790                                         | + 1532.2 |
| + 4406.0 | + 2430                                         | + 1332.2 | + 5072.0 | + 2800                                         | + 1537.8 |
| + 4424.0 | + 2440                                         | + 1337.8 | + 5090.0 | + 2810                                         | + 1543.3 |
| + 4442.0 | + 2450                                         | + 1343.3 | + 5108.0 | + 2820                                         | + 1548.9 |
| + 4460.0 | + 2460                                         | + 1348.9 | + 5126.0 | + 2830                                         | + 1554.4 |
| + 4478.0 | + 2470                                         | + 1354.4 | + 5144.0 | + 2840                                         | + 1560.0 |
| + 4496.0 | + 2480                                         | + 1360.0 | + 5162.0 | + 2850                                         | + 1565.6 |
| + 4514.0 | + 2490                                         | + 1365.6 | + 5180.0 | + 2860                                         | + 1571.1 |
| + 4532.0 | + 2500                                         | + 1371.1 | + 5198.0 | + 2870                                         | + 1576.7 |
| + 4550.0 | + 2510                                         | + 1376.7 | + 5216.0 | + 2880                                         | + 1582.2 |
| + 4568.0 | + 2520                                         | + 1382.2 | + 5234.0 | + 2890                                         | + 1587.8 |
| + 4586.0 | + 2530                                         | + 1387.8 | + 5252.0 | + 2900                                         | + 1593.3 |
| + 4604.0 | + 2540                                         | + 1393.3 | + 5270.0 | + 2910                                         | + 1598.9 |
| + 4622.0 | + 2550                                         | + 1398.9 | + 5288.0 | + 2920                                         | + 1604.4 |
| + 4640.0 | + 2560                                         | + 1404.4 | + 5306.0 | + 2930                                         | + 1610.0 |
| + 4658.0 | + 2570                                         | + 1410.0 | + 5324.0 | + 2940                                         | + 1615.6 |
| + 4676.0 | + 2580                                         | + 1415.6 | + 5342.0 | + 2950                                         | + 1621.1 |
| + 4694.0 | + 2590                                         | + 1421.1 | + 5360.0 | + 2960                                         | + 1626.7 |
| + 4712.0 | + 2600                                         | + 1426.7 | + 5378.0 | + 2970                                         | + 1632.2 |
| + 4730.0 | + 2610                                         | + 1432.2 | + 5396.0 | + 2980                                         | + 1637.8 |
| + 4748.0 | + 2620                                         | + 1437.8 | + 5414.0 | + 2990                                         | + 1643.3 |
| + 4766.0 | + 2630                                         | + 1443.3 | + 5432.0 | + 3000                                         | + 1648.9 |
| + 4784.0 | + 2640                                         | + 1448.9 | + 5450.0 | + 3010                                         | + 1654.4 |
| + 4802.0 | + 2650                                         | + 1454.4 | + 5468.0 | + 3020                                         | + 1660.0 |
| + 4820.0 | + 2660                                         | + 1460.0 | + 5486.0 | + 3030                                         | + 1665.6 |
| + 4838.0 | + 2670                                         | + 1465.6 | + 5504.0 | + 3040                                         | + 1671.1 |
| + 4856.0 | + 2680                                         | + 1471.1 | + 5522.0 | + 3050                                         | + 1676.7 |
| + 4874.0 | + 2690                                         | + 1476.7 | + 5540.0 | + 3060                                         | + 1682.2 |
| + 4892.0 | + 2700                                         | + 1482.2 | + 5558.0 | + 3070                                         | + 1687.8 |
| + 4910.0 | + 2710                                         | + 1487.8 | + 5576.0 | + 3080                                         | + 1693.3 |
| + 4928.0 | + 2720                                         | + 1493.3 | + 5594.0 | + 3090                                         | + 1698.9 |
| + 4946.0 | + 2730                                         | + 1498.9 | + 5612.0 | + 3100                                         | + 1704.4 |

### 2.1.1 Conversion of Thermometer Scales

The following abbreviations are used: °F, degrees Fahrenheit; °C, degrees Celsius; °K, degrees Kelvin; °Ré, degrees Reaumur; °R, degrees Rankine; °Z, degrees on any scale; (fp)“Z”, the freezing point of water on the Z scale; and (bp)“Z”, the boiling point of water on the Z scale. Reference: Dodds, *Chemical and Metallurgical Engineering* **38**:476 (1931).

$$\frac{^{\circ}\text{F} - 32}{180} = \frac{^{\circ}\text{C}}{100} = \frac{^{\circ}\text{Ré}}{80} = \frac{\text{K} - 273}{100} = \frac{^{\circ}\text{R} - 492}{180} = \frac{^{\circ}\text{Z} - (\text{fp})\text{“Z”}}{(\text{bp})\text{“Z”} - (\text{fp})\text{“Z”}}$$

*Examples*

(1) To find the Fahrenheit temperature corresponding to  $-20^{\circ}\text{C}$ :

$$\frac{^{\circ}\text{F} - 32}{180} = \frac{^{\circ}\text{C}}{100} \quad \text{or} \quad \frac{^{\circ}\text{F} - 32}{180} = \frac{-20}{100}$$

$$^{\circ}\text{F} - 32 = \frac{(-20)(180)}{100} = -36$$

$$^{\circ}\text{F} = -4$$

(2) To find the Reaumur temperature corresponding to  $20^{\circ}\text{F}$ :

$$\frac{^{\circ}\text{F} - 32}{180} = \frac{^{\circ}\text{Ré}}{80} = \frac{20 - 32}{180} = \frac{^{\circ}\text{Ré}}{80}$$

$$\text{i.e.,} \quad 20^{\circ}\text{F} = -5.33^{\circ}\text{Ré}$$

(3) To find the correct temperature on a thermometer reading  $80^{\circ}\text{C}$  and that shows a reading of  $-0.30^{\circ}\text{C}$  in a melting ice/water mixture and  $99.0^{\circ}\text{C}$  in steam at 760 mm pressure of mercury:

$$\frac{^{\circ}\text{C}}{100} = \frac{\text{Z} - (\text{fp})\text{“Z”}}{(\text{bp})\text{“Z”} - (\text{fp})\text{“Z”}} = \frac{80 - (-0.30)}{99.0 - (-0.30)}$$

$$\text{i.e.,} \quad ^{\circ}\text{C} = 80.87 \quad (\text{corrected})$$

### 2.1.2 Density and Specific Gravity

**2.1.2.1 Hydrometers.** Various hydrometers and the relation between the various scales.

*Alcoholometer.* This hydrometer is used in determining the density of aqueous ethyl alcohol solutions; the reading in degrees is numerically the same as the percentage of alcohol by volume. The scale known as Tralle gives the percentage by volume. Wine and Must hydrometer relations are given below.

*Ammoniameter.* This hydrometer, employed in finding the density of aqueous ammonia solutions, has a scale graduated in equal divisions from  $0^{\circ}$  to  $40^{\circ}$ . To convert the reading to specific gravity multiply by 3 and subtract the resulting number from 1000.

*Balling Hydrometer.* See under Saccharometers.

*Barkometer or Barktrometer.* This hydrometer, which is used in determining the density of tanning liquors, has a scale from  $0^{\circ}$  to  $80^{\circ}\text{Bk}$ ; the number to the right of the decimal point of a specific gravity reading is the corresponding Bk degree; thus, a specific gravity of 1.015 is  $15^{\circ}\text{Bk}$ .

**Baumé Hydrometers.** For liquids heavier than water: This hydrometer was originally based on the density of a 10% sodium chloride solution, which was given the value of 10°, and the density of pure water, which was given the value of 0°; the interval between these two values was divided into 10 equal parts. Other reference points have been taken with the result that so much confusion exists that there are about 36 different scales in use, many of which are incorrect. In general a Baumé hydrometer should have inscribed on it the temperature at which it was calibrated and also the temperature of the water used in relating the density to a specific gravity. The following expression gives the relation between the specific gravity and several of the Baumé scales:

$$\text{Specific gravity} = \frac{m}{m - \text{Baumé}}$$

$$\begin{aligned} m &= 145 \text{ at } 60^{\circ}/60^{\circ}\text{F (15.56}^{\circ}\text{C)} && \text{for the American Scale} \\ &= 144 && \text{for the old scale used in Holland} \\ &= 146.3 \text{ at } 15^{\circ}\text{C} && \text{for the Gerlach Scale} \\ &= 144.3 \text{ at } 15^{\circ}\text{C} && \text{for the Rational Scale generally used in Germany} \end{aligned}$$

For liquids lighter than water: Originally the density of a solution of 1 gram of sodium chloride in 9 grams of water at 12.5°C was given a value of 10°Bé. The scale between these points was divided into ten equal parts and these divisions were repeated throughout the scale giving a relation which could be expressed by the formula: Specific gravity = 145.88/(135.88 + Bé), which is approximately equal to 146/(136 + Bé). Other scales have since come into more general use such as that of the Bureau of Standards in which the specific gravity at 60°/60°F = 140/(130 + Bé) and that of the American Petroleum Institute (A.P.I. Scale) in which the specific gravity at 60°/60°F = 141.5/(131.5 + API°).

See also special table for conversion to density and Twaddell scale.

**Beck's Hydrometer.** This hydrometer is graduated to show a reading of 0° in pure water and a reading of 30° in a solution with a specific gravity of 0.850, with equal scale divisions above and below these two points.

**Brix Hydrometer.** See under Saccharometers.

**Cartier's Hydrometer.** This hydrometer shows a reading of 22° when immersed in a solution having a density of 22° Baumé but the scale divisions are smaller than on the Baumé hydrometer in the ratio of 16 Cartier to 15 Baumé.

**Fatty Oil Hydrometer.** The graduations on this hydrometer are in specific gravity within the range 0.908 to 0.938. The letters on the scale correspond to the specific gravity of the various common oils as follows: *R*, rape; *O*, olive; *A*, almond; *S*, sesame; *HL*, hoof oil; *HP*, hemp; *C*, cotton seed; *L*, linseed. See also Oleometer below.

**Lactometers.** These hydrometers are used in determining the density of milk. The various scales in common use are the following:

*New York Board of Health* has a scale graduated into 120 equal parts, 0° being equal to the specific gravity of water and 100° being equal to a specific gravity of 1.029.

*Quevenne* lactometer is graduated from 15° to 40° corresponding to specific gravities from 1.015 to 1.040.

*Soxhlet* lactometer has a scale from 25° to 35° corresponding to specific gravities from 1.025 to 1.035 respectively.

*Oleometer.* A hydrometer for determining the density of vegetable and sperm oils with a scale from 50° to 0° corresponding to specific gravities from 0.870 to 0.970. See also Fatty Oil Hydrometer above.

*Saccharometers.* These hydrometers are used in determining the density of sugar solutions. Solutions of the same concentration but of different carbohydrates have very nearly the same specific gravity and in general a concentration of 10 grams of carbohydrate per 100 mL of solution shows a specific gravity of 1.0386. Thus, the wt. of sugar in 1000 mL soln. is (a) for conc. < 12g/100 mL: (wt. of 1000 mL soln. - 1000) ÷ 0.386; (b) for conc. > 12g/100 mL: (wt of 1000 mL soln. - 1000) ÷ 0.385.

*Brix* hydrometer is graduated so that the number of degrees is identical with the percentage by weight of cane sugar and is used at the temperature indicated on the hydrometer.

*Balling's* saccharometer is used in Europe and is practically identical with the Brix hydrometer.

*Bates* brewers' saccharometer which is used in determining the density of malt worts is graduated so that the divisions express pounds per barrel (32 gallons). The relation between degrees Bates (=b) and degrees Balling (=B) is shown by the following formula:  $B = 260b/(360 + b)$ .

See also below under Wine and Must Hydrometer.

*Salinometer.* This hydrometer, which is used in the pickling and meat packing plants, is graduated to show percentage of saturation of a sodium chloride solution. An aqueous solution is completely saturated when it contains 26.4% pure sodium chloride. The range from 0% to 26.4% is divided into 100 parts, each division therefore representing 1% of saturation. In another type of salinometer, the degrees correspond to percentages of sodium chloride expressed in grams of sodium chloride per 100 mL of water.

*Sprayometer (Parrot and Stewart).* This hydrometer which is used in determining the density of lime sulfur solutions has two scales; one scale is graduated from 0° to 38° Baumé and the other scale is from 1.000 to 1.350 specific gravity.

*Tralle Hydrometer.* See Alcoholometer above.

*Twaddell Hydrometer.* This hydrometer, which is used only for liquids heavier than water, has a scale such that when the reading is multiplied by 5 and added to 1000 the resulting number is the specific gravity with reference to water as 1000. To convert specific gravity at 60°/60°F to Twaddell degrees, take the decimal portion of the specific gravity value and multiply it by 200; thus a specific gravity of 1.032 =  $0.032 \times 200 = 6.4^\circ$  Tw. See also special table for conversion to density and Baumé scale.

*Wine and Must Hydrometer.* This instrument has three scales. One scale shows readings of 0° to 15° Brix for sugar (see Brix Hydrometer above); another scale from 0° to 15° Tralle is used for sweet wines to indicate the percentage of alcohol by volume; and a third scale from 0° to 20° Tralle is used for tart wines to indicate the percentage of alcohol by volume.

**2.1.2.2 Conversion of Specific Gravity at 25°/25°C to Density at any Temperature from 0° to 40°C.\*** Liquids change volume with change in temperature, but the amount of this change,  $\beta$  (coefficient of cubical expansion), varies widely with different liquids, and to some extent for the same liquid at different temperatures.

The table below, which is calculated from the relationship:

$$F_{\beta_t} = \frac{\text{density of water at } 25^\circ\text{C} (=0.99705)}{1 - \beta(25 - t)} \quad (2.1)$$

\* Cf. Dreisbach, *Ind. Eng. Chem., Anal. Ed.* 12:160 (1940).

may be used to find  $d^t$ , the density (weight of 1 mL) of a liquid at any temperature ( $t$ ) between  $0^\circ$  and  $40^\circ\text{C}$  if the specific gravity at  $25^\circ/25^\circ\text{C}$  ( $S$ ) and the coefficient of cubical expansion ( $\beta$ ) are known. Substitutions are made in the equations:

$$d^t = SF_{\beta_t} \tag{2.2}$$

$$S = \frac{d^t}{F_{\beta_t}} \tag{2.3}$$

Factors ( $F_{\beta_t}$ )

$Density\ t^\circ\text{C} = sp.\ gr.\ 25^\circ/25^\circ \times F_{\beta_t}$

| <div><div>°C.</div><div>*β × 10<sup>3</sup></div></div> | 0      | 5      | 10     | 15     | 20      | 25      | 30      | 35      | 40      |
|---------------------------------------------------------|--------|--------|--------|--------|---------|---------|---------|---------|---------|
| 1.3                                                     | 1.0306 | 1.0237 | 1.0169 | 1.0102 | 1.0036  | 0.99705 | 0.99065 | 0.9843  | 0.9780  |
| 1.2                                                     | 1.0279 | 1.0216 | 1.0154 | 1.0092 | 1.0031  | 0.99705 | 0.9911  | 0.9853  | 0.9794  |
| 1.1                                                     | 1.0253 | 1.0195 | 1.0138 | 1.0082 | 1.0026  | 0.99705 | 0.9916  | 0.9963  | 0.9809  |
| 1.0                                                     | 1.0227 | 1.0174 | 1.0123 | 1.0072 | 1.0021  | 0.99705 | 0.9921  | 0.9872  | 0.98234 |
| 0.9                                                     | 1.0200 | 1.0153 | 1.0107 | 1.0060 | 1.0016  | 0.99705 | 0.99262 | 0.9882  | 0.9838  |
| 0.8                                                     | 1.0174 | 1.0133 | 1.0092 | 1.0051 | 1.0011  | 0.99705 | 0.9931  | 0.98918 | 0.9851  |
| 0.7                                                     | 1.0148 | 1.0113 | 1.0077 | 1.0041 | 1.0006  | 0.99705 | 0.9935  | 0.99015 | 0.98672 |
| 0.6                                                     | 1.0122 | 1.0092 | 1.0061 | 1.0031 | 1.0001  | 0.99705 | 0.9941  | 0.9911  | 0.9882  |
| 0.5                                                     | 1.0097 | 1.0072 | 1.0046 | 1.0021 | 0.99958 | 0.99705 | 0.9944  | 0.9921  | 0.9897  |
| 0.                                                      | 1.0071 | 1.0051 | 1.0031 | 1.0011 | 0.99908 | 0.99705 | 0.9951  | 0.9931  | 0.9911  |

\*  $\beta$  = coefficient of cubical expansion.

*Examples.* All examples are based upon an assumed coefficient of cubical expansion,  $\beta$ , of  $1.3 \times 10^{-3}$ .

*Example 1.* To find the density of a liquid at  $20^\circ\text{C}$ ,  $d^{20}$ , which has a specific gravity ( $S$ ) of  $1.2500^{25}_{25}$ :

From the table above  $F_{\beta_t}$  at  $20^\circ\text{C} = 1.0036$ .

$$d^{20} = d^t = SF_{\beta_t} = 1.2500 \times 1.0036 = 1.2545$$

*Example 2.* To find the density at  $20^\circ\text{C}$  ( $d^{20}$ ) of a liquid which has a specific gravity of  $1.2500^{17}_{4}$ :

Since the density of water at  $4^\circ\text{C}$  is equal to 1, specific gravity at  $17^\circ/4^\circ = d^{17} = 1.2500$ .  
Substitution in Equation 3 with  $F_{\beta_t}$  at  $17^\circ\text{C}$ , by interpolation from the table, equal to 1.00756, gives

$$Sp.\ gr.\ 25^\circ/25^\circ = S = 1.2500 \div 1.00756$$

Substitution of this value for  $S$  in Equation 2 with  $F_{\beta_t}$  at  $20^\circ\text{C}$ , from the table, equal to 1.0036, gives

$$d^{20} = d^t = (1.2500 \div 1.00756) \times 1.0036 = 1.2451$$

*Example 3.* To find the specific gravity at  $20^{\circ}/4^{\circ}\text{C}$  of a liquid which has a specific gravity of  $1.2500_{\frac{25}{4}}$ :

Since the density of water at  $4^{\circ}\text{C}$ , is equal to 1, specific gravity  $25^{\circ}/4^{\circ} = d^{25} = 1.2500$ ; and, specific gravity  $20^{\circ}/4^{\circ} = d^{20}$ .

Substitution in Equation 3, with  $d^t = 1.2500$ ; and, with  $F_{\beta_t}$  at  $25^{\circ}\text{C}$ , from the table, equal to 0.99705, gives

$$\text{Sp. gr. } 25^{\circ}/25^{\circ} = S = 1.2500 \div 0.99705$$

Substitution of this value for  $S$  in Equation 2, with  $F_{\beta_t}$  at  $20^{\circ}\text{C}$ , from the table, equal to 1.0036, gives

$$\text{Sp. gr. } 20^{\circ}/4^{\circ} = d^{20} = (1.2500 \div 0.99705) \times 1.0036 = 1.2582$$

*Example 4.* To find the density at  $25^{\circ}\text{C}$  of a liquid which has a specific gravity of  $1.2500_{\frac{15}{15}}$ :

Since the density of water at  $15^{\circ}\text{C} = 0.99910$ ,

$$d^{15} = \text{sp. gr. } 15^{\circ}/15^{\circ} \times 0.99910 = 1.2500 \times 0.99910$$

Substitution in Equation 3, with  $F_{\beta_t}$  at  $15^{\circ}\text{C}$ , from the table, equal to 1.0102, gives

$$\text{Sp. gr. } 25^{\circ}/25^{\circ} = S = (1.2500 \times 0.99910) \div 1.0102$$

Substitution of this value for  $S$  in Equation 2, with  $F_{\beta_t}$  at  $25^{\circ}$ , from the table, equal to 0.99705, gives

$$d^{26} = d^t = (1.2500 \times 0.99910 \div 1.0102) \times 0.99705 = 1.2326$$

### 2.1.3 Barometry and Barometric Corrections

In principle, the mercurial barometer balances a column of pure mercury against the weight of the atmosphere. The height of the column above the level of the mercury in the reservoir can be measured and serves as a direct index of atmospheric pressure. The space above the mercury in a barometer tube should be a Torricellian vacuum, perfect except for the practically negligible vapor pressure of mercury. The perfection of the vacuum is indicated by the sharpness of the click noted when the barometer tube is inclined. A barometer should be in a vertical position, suspended rather than fastened to a wall, and in a good light but not exposed to direct sunlight or too near a source of heat. The standard conditions for barometric measurements are  $0^{\circ}\text{C}$  and gravity as at  $45^{\circ}$  latitude and sea level. There are numerous sources of error, but corrections for most of these are readily applied. Some of the corrections are very small, and their application may be questionable in view of the probably larger errors. The degree of consistency to be expected in careful measurements is about 0.13 mm with a 6.4-mm tube, increasing to 0.04 mm with a tube 12.7 mm in diameter.

In reading a barometer of the Fortin type (the usual laboratory instrument for precision measurements), the procedure should be as follows: (1) Observe and record the temperature as indicated by the thermometer attached to the barometer. The temperature correction is very important and may be affected by heat from the observer's body. (2) Set the mercury in the reservoir at zero level, so that the point of the pin above the mercury just touches the surface, making a barely noticeable dimple therein. Tap the tube at the top and verify the zero setting. (3) Bring the vernier down until the view at the light background is cut off at the highest point of the meniscus. Record the reading.

The corrections to be made on the reading are as follows: (1) Temperature, to correct for the difference in thermal expansion of the mercury and the brass (or glass) to which the scale is attached.

This correction converts the reading into the value of 0°C. The brass scale table is applicable to the Fortin barometer. See Tables 2.10 latitude-gravity correction, and 2.11 altitude-gravity correction, to compensate for differences in gravity, which would affect the height of the mercury column by variation in mass. If local gravity is unknown, an approximate correction may be made from the tables. Local values of gravity are often subject to irregularities which lead to errors even when the corrections here provided are made. It is, therefore, advisable to determine the local value of gravity, from which the correction can be effected in the following manner:

$$Bt = Br + \left( \frac{g_1 - g_0}{g_0} \right) \times Br$$

in which  $Bt$  and  $Br$  are the true and the observed heights of the barometer, respectively.  $g_0$  is standard gravity ( $980\,665\text{ cm} \cdot \text{s}^{-2}$ ), and  $g_1$  is the local gravity. It may be noted that for most localities,  $g_1$  is smaller than  $g_0$ , which makes the correction negative. These corrections compensate the reading to gravity at 45° latitude and sea level. (3) Correction for capillary depression of the level of the meniscus. This varies with the tube diameter and actual height of the meniscus in a particular case. Some barometers are calibrated to allow for an average value of the latter and approximating the correction. See table. (4) Correction for vapor pressure of mercury. This correction is usually negligible, being only 0.001 mm at 20°C and 0.006 mm at 40°C. This correction is added. See table of vapor pressure of mercury.

The corrections above do not apply to aneroid barometers. These instruments should be calibrated at regular intervals by checking them against a corrected mercurial barometer.

For records on weather maps, meteorologists customarily correct barometer readings to sea level, and some barometers may be calibrated accordingly. Such instruments are not suitable for laboratory use where true pressure under standard conditions is required. Scale corrections should be specified in the maker's instructions with the instrument, and are also indicated by the lack of correspondence between a gauge mark usually placed exactly 76.2 cm from the zero point and the 76.2-cm scale graduation.

**TABLE 2.9** Barometer Temperature Correction—Metric Units

The values in the table below are to be subtracted from the observed readings to correct for the difference in the expansion of the mercury and the glass scale at different temperatures.

| A. Glass scale |                                          |      |      |      |      |      |      |
|----------------|------------------------------------------|------|------|------|------|------|------|
| Temp.<br>°C.   | Observed barometer height in millimeters |      |      |      |      |      |      |
|                | 700                                      | 730  | 740  | 750  | 760  | 770  | 800  |
|                | mm.                                      | mm.  | mm.  | mm.  | mm.  | mm.  | mm.  |
| 0              | 0.00                                     | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 1              | 0.12                                     | 0.13 | 0.13 | 0.13 | 0.13 | 0.13 | 0.14 |
| 2              | 0.24                                     | 0.25 | 0.26 | 0.26 | 0.26 | 0.27 | 0.27 |
| 3              | 0.36                                     | 0.38 | 0.38 | 0.39 | 0.40 | 0.40 | 0.42 |
| 4              | 0.49                                     | 0.51 | 0.51 | 0.52 | 0.53 | 0.53 | 0.55 |
| 5              | 0.61                                     | 0.63 | 0.64 | 0.65 | 0.66 | 0.67 | 0.69 |
| 6              | 0.73                                     | 0.76 | 0.77 | 0.78 | 0.79 | 0.80 | 0.83 |
| 7              | 0.85                                     | 0.89 | 0.90 | 0.91 | 0.92 | 0.93 | 0.97 |
| 8              | 0.97                                     | 1.01 | 1.03 | 1.04 | 1.05 | 1.07 | 1.11 |
| 9              | 1.09                                     | 1.14 | 1.15 | 1.17 | 1.18 | 1.20 | 1.25 |
| 10             | 1.21                                     | 1.26 | 1.28 | 1.30 | 1.32 | 1.33 | 1.39 |
| 11             | 1.33                                     | 1.39 | 1.41 | 1.43 | 1.45 | 1.47 | 1.52 |
| 12             | 1.45                                     | 1.52 | 1.54 | 1.56 | 1.58 | 1.60 | 1.66 |
| 13             | 1.58                                     | 1.64 | 1.67 | 1.69 | 1.71 | 1.73 | 1.80 |
| 14             | 1.70                                     | 1.77 | 1.79 | 1.82 | 1.84 | 1.87 | 1.94 |
| 15             | 1.82                                     | 1.90 | 1.92 | 1.95 | 1.97 | 2.00 | 2.08 |
| 16             | 1.94                                     | 2.02 | 2.05 | 2.08 | 2.10 | 2.13 | 2.21 |
| 17             | 2.06                                     | 2.15 | 2.18 | 2.21 | 2.23 | 2.26 | 2.35 |
| 18             | 2.18                                     | 2.27 | 2.30 | 2.33 | 2.37 | 2.40 | 2.49 |
| 19             | 2.30                                     | 2.40 | 2.43 | 2.46 | 2.50 | 2.53 | 2.63 |
| 20             | 2.42                                     | 2.52 | 2.56 | 2.59 | 2.63 | 2.66 | 2.77 |
| 21             | 2.54                                     | 2.65 | 2.69 | 2.72 | 2.76 | 2.79 | 2.90 |
| 22             | 2.66                                     | 2.78 | 2.81 | 2.85 | 2.89 | 2.93 | 3.04 |
| 23             | 2.78                                     | 2.90 | 2.94 | 2.98 | 3.02 | 3.06 | 3.18 |
| 24             | 2.90                                     | 3.03 | 3.07 | 3.11 | 3.15 | 3.19 | 3.32 |
| 25             | 3.02                                     | 3.15 | 3.20 | 3.24 | 3.28 | 3.32 | 3.45 |
| 26             | 3.14                                     | 3.28 | 3.32 | 3.37 | 3.41 | 3.46 | 3.59 |
| 27             | 3.26                                     | 3.40 | 3.45 | 3.50 | 3.54 | 3.59 | 3.73 |
| 28             | 3.38                                     | 3.53 | 3.58 | 3.63 | 3.67 | 3.72 | 3.87 |
| 29             | 3.50                                     | 3.65 | 3.70 | 3.75 | 3.80 | 3.85 | 4.00 |
| 30             | 3.62                                     | 3.78 | 3.83 | 3.88 | 3.93 | 3.99 | 4.14 |
| 31             | 3.74                                     | 3.90 | 3.96 | 4.01 | 4.06 | 4.12 | 4.28 |
| 32             | 3.86                                     | 4.03 | 4.08 | 4.14 | 4.20 | 4.25 | 4.42 |
| 33             | 3.98                                     | 4.15 | 4.21 | 4.27 | 4.33 | 4.38 | 4.55 |
| 34             | 4.10                                     | 4.28 | 4.34 | 4.40 | 4.46 | 4.51 | 4.69 |
| 35             | 4.22                                     | 4.40 | 4.47 | 4.53 | 4.59 | 4.65 | 4.83 |



**TABLE 2.9** Barometer Temperature Correction—Metric Units (*Continued*)

The values in the table below are to be subtracted from the observed readings to correct for the difference in the expansion of the mercury and the glass scale at different temperatures.

| B. Brass scale |                                          |      |      |      |      |      |      |
|----------------|------------------------------------------|------|------|------|------|------|------|
| Temp.<br>°C.   | Observed barometer height in millimeters |      |      |      |      |      |      |
|                | 640                                      | 650  | 660  | 670  | 680  | 690  | 700  |
|                | mm.                                      | mm.  | mm.  | mm.  | mm.  | mm.  | mm.  |
| 0              | 0.00                                     | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 1              | 0.10                                     | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 |
| 2              | 0.21                                     | 0.21 | 0.22 | 0.22 | 0.22 | 0.23 | 0.23 |
| 3              | 0.31                                     | 0.32 | 0.32 | 0.33 | 0.33 | 0.34 | 0.34 |
| 4              | 0.42                                     | 0.42 | 0.43 | 0.44 | 0.44 | 0.45 | 0.46 |
| 5              | 0.52                                     | 0.53 | 0.54 | 0.55 | 0.55 | 0.56 | 0.57 |
| 6              | 0.63                                     | 0.64 | 0.65 | 0.66 | 0.66 | 0.67 | 0.68 |
| 7              | 0.73                                     | 0.74 | 0.75 | 0.76 | 0.78 | 0.79 | 0.80 |
| 8              | 0.84                                     | 0.85 | 0.86 | 0.87 | 0.89 | 0.90 | 0.91 |
| 9              | 0.94                                     | 0.95 | 0.97 | 0.98 | 1.00 | 1.01 | 1.03 |
| 10             | 1.04                                     | 1.06 | 1.07 | 1.09 | 1.11 | 1.12 | 1.14 |
| 11             | 1.15                                     | 1.16 | 1.18 | 1.20 | 1.22 | 1.24 | 1.25 |
| 12             | 1.25                                     | 1.27 | 1.29 | 1.31 | 1.33 | 1.35 | 1.37 |
| 13             | 1.35                                     | 1.38 | 1.40 | 1.42 | 1.44 | 1.46 | 1.48 |
| 14             | 1.46                                     | 1.48 | 1.50 | 1.53 | 1.55 | 1.57 | 1.59 |
| 15             | 1.56                                     | 1.59 | 1.61 | 1.64 | 1.66 | 1.68 | 1.71 |
| 16             | 1.67                                     | 1.69 | 1.72 | 1.74 | 1.77 | 1.80 | 1.82 |
| 17             | 1.77                                     | 1.80 | 1.82 | 1.85 | 1.88 | 1.91 | 1.94 |
| 18             | 1.87                                     | 1.90 | 1.93 | 1.96 | 1.99 | 2.02 | 2.05 |
| 19             | 1.98                                     | 2.01 | 2.04 | 2.07 | 2.10 | 2.13 | 2.16 |
| 20             | 2.08                                     | 2.11 | 2.15 | 2.18 | 2.21 | 2.24 | 2.28 |
| 21             | 2.18                                     | 2.22 | 2.25 | 2.29 | 2.32 | 2.35 | 2.39 |
| 22             | 2.29                                     | 2.32 | 2.36 | 2.40 | 2.43 | 2.47 | 2.50 |
| 23             | 2.39                                     | 2.43 | 2.47 | 2.50 | 2.54 | 2.58 | 2.62 |
| 24             | 2.49                                     | 2.53 | 2.57 | 2.61 | 2.65 | 2.69 | 2.73 |
| 25             | 2.60                                     | 2.64 | 2.68 | 2.72 | 2.76 | 2.80 | 2.84 |
| 26             | 2.70                                     | 2.74 | 2.79 | 2.83 | 2.87 | 2.91 | 2.96 |
| 27             | 2.81                                     | 2.85 | 2.89 | 2.94 | 2.98 | 3.02 | 3.07 |
| 28             | 2.91                                     | 2.95 | 3.00 | 3.05 | 3.09 | 3.14 | 3.18 |
| 29             | 3.01                                     | 3.06 | 3.11 | 3.15 | 3.20 | 3.25 | 3.29 |
| 30             | 3.12                                     | 3.16 | 3.21 | 3.26 | 3.31 | 3.36 | 3.41 |
| 31             | 3.22                                     | 3.27 | 3.32 | 3.37 | 3.42 | 3.47 | 3.52 |
| 32             | 3.32                                     | 3.37 | 3.43 | 3.48 | 3.53 | 3.58 | 3.63 |
| 33             | 3.42                                     | 3.48 | 3.53 | 3.59 | 3.64 | 3.69 | 3.75 |
| 34             | 3.53                                     | 3.58 | 3.64 | 3.69 | 3.75 | 3.80 | 3.86 |
| 35             | 3.63                                     | 3.69 | 3.74 | 3.80 | 3.86 | 3.91 | 3.97 |

TABLE 2.9 Barometer Temperature Correction—Metric Units (Continued)

| B. Brass scale (continued)               |      |      |      |      |      |      |      |              |
|------------------------------------------|------|------|------|------|------|------|------|--------------|
| Observed barometer height in millimeters |      |      |      |      |      |      |      | Temp.<br>°C. |
| 710                                      | 720  | 730  | 740  | 750  | 760  | 770  | 780  |              |
| mm.                                      | mm.  | mm.  | mm.  | mm.  | mm.  | mm.  | mm.  |              |
| 0.00                                     | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0            |
| 0.12                                     | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 | 0.13 | 0.13 | 1            |
| 0.23                                     | 0.23 | 0.24 | 0.24 | 0.24 | 0.25 | 0.25 | 0.25 | 2            |
| 0.35                                     | 0.35 | 0.36 | 0.36 | 0.37 | 0.37 | 0.38 | 0.38 | 3            |
| 0.46                                     | 0.47 | 0.48 | 0.48 | 0.49 | 0.50 | 0.50 | 0.51 | 4            |
| 0.58                                     | 0.59 | 0.59 | 0.60 | 0.61 | 0.62 | 0.63 | 0.64 | 5            |
| 0.69                                     | 0.70 | 0.71 | 0.72 | 0.73 | 0.74 | 0.75 | 0.76 | 6            |
| 0.81                                     | 0.82 | 0.83 | 0.84 | 0.86 | 0.87 | 0.88 | 0.89 | 7            |
| 0.93                                     | 0.94 | 0.95 | 0.96 | 0.98 | 0.99 | 1.00 | 1.02 | 8            |
| 1.04                                     | 1.06 | 1.07 | 1.08 | 1.10 | 1.11 | 1.13 | 1.14 | 9            |
| 1.16                                     | 1.17 | 1.19 | 1.21 | 1.22 | 1.24 | 1.25 | 1.27 | 10           |
| 1.27                                     | 1.29 | 1.31 | 1.33 | 1.34 | 1.36 | 1.38 | 1.40 | 11           |
| 1.39                                     | 1.41 | 1.43 | 1.45 | 1.47 | 1.48 | 1.50 | 1.52 | 12           |
| 1.50                                     | 1.52 | 1.54 | 1.57 | 1.59 | 1.61 | 1.63 | 1.65 | 13           |
| 1.62                                     | 1.64 | 1.66 | 1.69 | 1.71 | 1.73 | 1.75 | 1.78 | 14           |
| 1.73                                     | 1.76 | 1.78 | 1.81 | 1.83 | 1.85 | 1.88 | 1.90 | 15           |
| 1.85                                     | 1.87 | 1.90 | 1.93 | 1.95 | 1.98 | 2.00 | 2.03 | 16           |
| 1.96                                     | 1.99 | 2.02 | 2.05 | 2.07 | 2.10 | 2.13 | 2.16 | 17           |
| 2.08                                     | 2.11 | 2.14 | 2.17 | 2.20 | 2.22 | 2.25 | 2.28 | 18           |
| 2.19                                     | 2.22 | 2.25 | 2.29 | 2.32 | 2.35 | 2.38 | 2.41 | 19           |
| 2.31                                     | 2.34 | 2.37 | 2.41 | 2.44 | 2.47 | 2.50 | 2.54 | 20           |
| 2.42                                     | 2.46 | 2.49 | 2.53 | 2.56 | 2.59 | 2.63 | 2.66 | 21           |
| 2.54                                     | 2.57 | 2.61 | 2.65 | 2.68 | 2.72 | 2.75 | 2.79 | 22           |
| 2.65                                     | 2.69 | 2.73 | 2.77 | 2.80 | 2.84 | 2.88 | 2.91 | 23           |
| 2.77                                     | 2.81 | 2.85 | 2.88 | 2.92 | 2.96 | 3.00 | 3.04 | 24           |
| 2.88                                     | 2.92 | 2.96 | 3.00 | 3.05 | 3.09 | 3.13 | 3.17 | 25           |
| 3.00                                     | 3.04 | 3.08 | 3.12 | 3.17 | 3.21 | 3.25 | 3.29 | 26           |
| 3.11                                     | 3.16 | 3.20 | 3.24 | 3.29 | 3.33 | 3.38 | 3.42 | 27           |
| 3.23                                     | 3.27 | 3.32 | 3.36 | 3.41 | 3.45 | 3.50 | 3.54 | 28           |
| 3.34                                     | 3.39 | 3.44 | 3.48 | 3.53 | 3.58 | 3.62 | 3.67 | 29           |
| 3.46                                     | 3.50 | 3.55 | 3.60 | 3.65 | 3.70 | 3.75 | 3.80 | 30           |
| 3.57                                     | 3.62 | 3.67 | 3.72 | 3.77 | 3.82 | 3.87 | 3.92 | 31           |
| 3.68                                     | 3.74 | 3.79 | 3.84 | 3.89 | 3.94 | 4.00 | 4.05 | 32           |
| 3.80                                     | 3.85 | 3.91 | 3.96 | 4.01 | 4.07 | 4.12 | 4.17 | 33           |
| 3.91                                     | 3.97 | 4.02 | 4.08 | 4.13 | 4.19 | 4.24 | 4.30 | 34           |
| 4.03                                     | 4.09 | 4.14 | 4.20 | 4.26 | 4.31 | 4.37 | 4.43 | 35           |

TABLE 2.9 Barometer Temperature Correction—Metric Units (Continued)

| C. Correction of a barometer for capillarity (Smithsonian Tables) |                                       |      |      |      |      |      |      |      |
|-------------------------------------------------------------------|---------------------------------------|------|------|------|------|------|------|------|
| Diameter<br>of tube,<br>millimeters                               | Height of meniscus in millimeters     |      |      |      |      |      |      |      |
|                                                                   | 0.4                                   | 0.6  | 0.8  | 1.0  | 1.2  | 1.4  | 1.6  | 1.8  |
|                                                                   | Correction to be added in millimeters |      |      |      |      |      |      |      |
| 4                                                                 | 0.83                                  | 1.22 | 1.54 | 1.98 | 2.37 | .... | .... | .... |
| 5                                                                 | 0.47                                  | 0.65 | 0.86 | 1.19 | 1.45 | 1.80 | .... | .... |
| 6                                                                 | 0.27                                  | 0.41 | 0.56 | 0.78 | 0.98 | 1.21 | 1.43 | .... |
| 7                                                                 | 0.18                                  | 0.28 | 0.40 | 0.53 | 0.67 | 0.82 | 0.97 | 1.13 |
| 8                                                                 | ....                                  | 0.20 | 0.29 | 0.38 | 0.46 | 0.56 | 0.65 | 0.77 |
| 9                                                                 | ....                                  | 0.15 | 0.21 | 0.28 | 0.33 | 0.40 | 0.46 | 0.52 |
| 10                                                                | ....                                  | .... | 0.15 | 0.20 | 0.25 | 0.29 | 0.33 | 0.37 |
| 11                                                                | ....                                  | .... | 0.10 | 0.14 | 0.18 | 0.21 | 0.24 | 0.27 |
| 12                                                                | ....                                  | .... | 0.07 | 0.10 | 0.13 | 0.15 | 0.18 | 0.19 |
| 13                                                                | ....                                  | .... | 0.04 | 0.07 | 0.10 | 0.12 | 0.13 | 0.14 |

TABLE 2.10 Barometric Latitude-Gravity Table—Metric Units

Smithsonian Tables.

The values in the table below are to be subtracted from the barometric reading for latitudes from 0 to 45° inclusive, and are to be added from 46 to 90°.

| Deg.<br>Lat. | Barometer readings, millimeters |      |      |      |      |      |
|--------------|---------------------------------|------|------|------|------|------|
|              | 680                             | 700  | 720  | 740  | 760  | 780  |
|              | mm.                             | mm.  | mm.  | mm.  | mm.  | mm.  |
| 0            | 1.82                            | 1.87 | 1.93 | 1.98 | 2.04 | 2.09 |
| 5            | 1.79                            | 1.85 | 1.90 | 1.95 | 2.00 | 2.06 |
| 10           | 1.71                            | 1.76 | 1.81 | 1.86 | 1.92 | 1.97 |
| 15           | 1.58                            | 1.63 | 1.67 | 1.72 | 1.77 | 1.81 |
| 20           | 1.40                            | 1.44 | 1.49 | 1.53 | 1.57 | 1.61 |
| 21           | 1.36                            | 1.40 | 1.44 | 1.48 | 1.52 | 1.56 |
| 22           | 1.32                            | 1.36 | 1.40 | 1.44 | 1.48 | 1.51 |
| 23           | 1.28                            | 1.31 | 1.35 | 1.39 | 1.43 | 1.46 |
| 24           | 1.23                            | 1.27 | 1.30 | 1.34 | 1.37 | 1.41 |
| 25           | 1.18                            | 1.22 | 1.25 | 1.29 | 1.32 | 1.36 |
| 26           | 1.13                            | 1.17 | 1.20 | 1.23 | 1.27 | 1.30 |
| 27           | 1.08                            | 1.12 | 1.15 | 1.18 | 1.21 | 1.24 |
| 28           | 1.03                            | 1.06 | 1.09 | 1.12 | 1.15 | 1.18 |
| 29           | 0.98                            | 1.01 | 1.04 | 1.07 | 1.10 | 1.12 |
| 30           | 0.93                            | 0.95 | 0.98 | 1.01 | 1.04 | 1.06 |
| 31           | 0.87                            | 0.90 | 0.92 | 0.95 | 0.98 | 1.00 |
| 32           | 0.82                            | 0.84 | 0.86 | 0.89 | 0.91 | 0.94 |
| 33           | 0.76                            | 0.78 | 0.80 | 0.83 | 0.85 | 0.87 |
| 34           | 0.70                            | 0.72 | 0.74 | 0.76 | 0.79 | 0.81 |
| 35           | 0.64                            | 0.66 | 0.68 | 0.70 | 0.72 | 0.74 |
| 36           | 0.58                            | 0.60 | 0.62 | 0.64 | 0.65 | 0.67 |
| 37           | 0.52                            | 0.54 | 0.56 | 0.57 | 0.59 | 0.60 |
| 38           | 0.46                            | 0.48 | 0.49 | 0.51 | 0.52 | 0.53 |

**TABLE 2.10** Barometric Latitude-Gravity Table—Metric Units (*Continued*)

| Deg.<br>Lat. | Barometer readings, millimeters |      |      |      |      |      |
|--------------|---------------------------------|------|------|------|------|------|
|              | 680                             | 700  | 720  | 740  | 760  | 780  |
|              | mm.                             | mm.  | mm.  | mm.  | mm.  | mm.  |
| 39           | 0.40                            | 0.42 | 0.43 | 0.44 | 0.45 | 0.46 |
| 40           | 0.34                            | 0.35 | 0.36 | 0.37 | 0.38 | 0.39 |
| 41           | 0.28                            | 0.29 | 0.30 | 0.30 | 0.31 | 0.32 |
| 42           | 0.22                            | 0.22 | 0.23 | 0.24 | 0.24 | 0.25 |
| 43           | 0.16                            | 0.16 | 0.16 | 0.17 | 0.17 | 0.18 |
| 44           | 0.09                            | 0.10 | 0.10 | 0.10 | 0.10 | 0.11 |
| 45           | 0.03                            | 0.03 | 0.03 | 0.03 | 0.03 | 0.04 |
| 46           | 0.03                            | 0.03 | 0.03 | 0.03 | 0.04 | 0.04 |
| 47           | 0.09                            | 0.10 | 0.10 | 0.10 | 0.10 | 0.11 |
| 48           | 0.16                            | 0.16 | 0.17 | 0.17 | 0.18 | 0.18 |
| 49           | 0.22                            | 0.23 | 0.23 | 0.24 | 0.25 | 0.25 |
| 50           | 0.28                            | 0.29 | 0.30 | 0.31 | 0.31 | 0.32 |
| 51           | 0.34                            | 0.35 | 0.36 | 0.37 | 0.38 | 0.39 |
| 52           | 0.40                            | 0.42 | 0.43 | 0.44 | 0.45 | 0.46 |
| 53           | 0.46                            | 0.48 | 0.49 | 0.51 | 0.52 | 0.53 |
| 54           | 0.52                            | 0.54 | 0.56 | 0.57 | 0.59 | 0.60 |
| 55           | 0.58                            | 0.60 | 0.62 | 0.64 | 0.65 | 0.67 |
| 56           | 0.64                            | 0.66 | 0.68 | 0.70 | 0.72 | 0.74 |
| 57           | 0.70                            | 0.72 | 0.74 | 0.76 | 0.78 | 0.80 |
| 58           | 0.76                            | 0.78 | 0.80 | 0.82 | 0.85 | 0.87 |
| 59           | 0.81                            | 0.84 | 0.86 | 0.89 | 0.91 | 0.93 |
| 60           | 0.87                            | 0.89 | 0.92 | 0.94 | 0.97 | 1.00 |
| 61           | 0.92                            | 0.95 | 0.98 | 1.00 | 1.03 | 1.06 |
| 62           | 0.97                            | 1.00 | 1.02 | 1.05 | 1.08 | 1.11 |
| 63           | 1.03                            | 1.06 | 1.09 | 1.12 | 1.15 | 1.18 |
| 64           | 1.08                            | 1.11 | 1.14 | 1.17 | 1.20 | 1.23 |
| 65           | 1.13                            | 1.16 | 1.19 | 1.22 | 1.26 | 1.29 |
| 66           | 1.17                            | 1.21 | 1.24 | 1.28 | 1.31 | 1.35 |
| 67           | 1.22                            | 1.25 | 1.29 | 1.33 | 1.36 | 1.40 |
| 68           | 1.26                            | 1.30 | 1.34 | 1.37 | 1.41 | 1.45 |
| 69           | 1.31                            | 1.34 | 1.38 | 1.42 | 1.46 | 1.50 |
| 70           | 1.35                            | 1.39 | 1.43 | 1.47 | 1.51 | 1.55 |
| 72           | 1.42                            | 1.47 | 1.51 | 1.55 | 1.59 | 1.63 |
| 75           | 1.53                            | 1.57 | 1.62 | 1.66 | 1.71 | 1.75 |
| 80           | 1.66                            | 1.71 | 1.76 | 1.81 | 1.86 | 1.90 |
| 85           | 1.74                            | 1.79 | 1.84 | 1.90 | 1.95 | 2.00 |
| 90           | 1.77                            | 1.82 | 1.87 | 1.93 | 1.98 | 2.03 |

**TABLE 2.11** Barometric Correction for Gravity—Metric Units

The values in the table below are to be subtracted from the readings taken on a mercurial barometer to correct for the decrease in gravity with increase in altitude.

[illegible]

**TABLE 2.12** Reduction of the Barometer to Sea Level—Metric Units

A barometer located at an elevation above sea level will show a reading lower than a barometer at sea level by an amount approximately 2.5 mm (0.1 in) for each 30.5 m (100 ft) of elevation. A closer approximation can be made by reference to the following tables, which take into account (1) the effect of altitude of the station at which the barometer is read, (2) the mean temperature of the air column extending from the station down to sea level, (3) the latitude of the station at which the barometer is read, and (4) the reading of the barometer corrected for its temperature, a correction which is applied only to mercurial barometers since the aneroid barometers are compensated for temperature effects.

*Example.* A barometer which has been corrected for its temperature reads 650 mm at a station whose altitude is 1350 m above sea level and at a latitude of 30°. The mean temperature (outdoor temperature) at the station is 20°C.

Table A (metric units) gives for these conditions a temperature-altitude factor of ..... 135.2  
The Latitude Factor Table gives for 135.2 at 30° lat. a correction of ..... +0.17  
Therefore, the corrected value of the temperature-altitude factor is ..... 135.37

Entering Table B (metric units), with a temperature-altitude factor of 135.37 and a barometric reading of 650 mm (corrected for temperature), the correction is found to be ..... 109.6  
Accordingly the barometric reading reduced to sea level is 650 + 109.6 = 759.6 mm.

**Latitude Factor—English or Metric Units.** For latitudes 0°–45° add the latitude factor, for 45°–90° subtract the latitude factor, from the values obtained in Table A.

| Temp.—Alt.<br>Factor<br>From Table A | Latitude |     |     |     |     |
|--------------------------------------|----------|-----|-----|-----|-----|
|                                      | 0°       | 10° | 20° | 30° | 45° |
| 50                                   | 0.1      | 0.1 | 0.1 | 0.1 | 0.0 |
| 100                                  | 0.3      | 0.3 | 0.2 | 0.1 | 0.0 |
| 150                                  | 0.4      | 0.4 | 0.3 | 0.2 | 0.0 |
| 200                                  | 0.5      | 0.5 | 0.4 | 0.3 | 0.0 |
| 250                                  | 0.7      | 0.6 | 0.5 | 0.3 | 0.0 |
| 300                                  | 0.8      | 0.8 | 0.6 | 0.4 | 0.0 |
| 350                                  | 0.9      | 0.9 | 0.7 | 0.5 | 0.0 |
|                                      | 90°      | 80° | 70° | 60° | 45° |

A. Values of the temperature-altitude factor for use in Table B.\*

| Altitude<br>in<br>Meters | Mean Temperature of Air Column in Centigrade Degrees |      |      |      |      |      |      |      |      |      |      |
|--------------------------|------------------------------------------------------|------|------|------|------|------|------|------|------|------|------|
|                          | –16°                                                 | –8°  | –4°  | 0°   | 6°   | 10°  | 14°  | 18°  | 20°  | 22°  | 26°  |
| 10                       | 1.2                                                  | 1.1  | 1.1  | 1.1  | 1.1  | 1.0  | 1.0  | 1.0  | 1.0  | 1.0  | 1.0  |
| 50                       | 5.8                                                  | 5.6  | 5.5  | 5.4  | 5.3  | 5.2  | 5.1  | 5.0  | 5.0  | 5.0  | 4.9  |
| 100                      | 11.5                                                 | 11.2 | 11.0 | 10.8 | 10.6 | 10.4 | 10.3 | 10.1 | 10.0 | 9.9  | 9.8  |
| 150                      | 17.3                                                 | 16.7 | 16.5 | 16.2 | 15.9 | 15.6 | 15.4 | 15.1 | 15.0 | 14.9 | 14.7 |
| 200                      | 23.0                                                 | 22.3 | 22.0 | 21.6 | 21.1 | 20.8 | 20.5 | 20.2 | 20.0 | 19.9 | 19.6 |
| 250                      | 28.8                                                 | 27.9 | 27.5 | 27.0 | 26.4 | 26.0 | 25.6 | 25.2 | 25.0 | 24.9 | 24.5 |
| 300                      | 34.5                                                 | 33.5 | 33.0 | 32.5 | 31.7 | 31.2 | 30.7 | 30.3 | 30.1 | 29.8 | 29.4 |
| 350                      | 40.3                                                 | 39.0 | 38.5 | 37.9 | 37.0 | 36.4 | 35.9 | 35.3 | 35.1 | 34.8 | 34.3 |
| 400                      | 46.0                                                 | 44.6 | 43.9 | 43.3 | 42.3 | 41.6 | 41.0 | 40.4 | 40.1 | 39.8 | 39.2 |
| 450                      | 51.8                                                 | 51.3 | 49.4 | 48.7 | 47.6 | 46.8 | 46.1 | 45.4 | 45.1 | 44.8 | 44.1 |
| 500                      | 57.5                                                 | 55.8 | 54.9 | 54.1 | 52.9 | 52.0 | 51.2 | 50.5 | 50.1 | 49.7 | 49.0 |
| 550                      | 63.3                                                 | 61.4 | 60.4 | 59.5 | 58.1 | 57.2 | 56.4 | 55.5 | 55.1 | 54.7 | 53.9 |
| 600                      | 69.0                                                 | 66.9 | 65.9 | 64.9 | 63.4 | 62.4 | 61.5 | 60.6 | 60.1 | 59.7 | 58.8 |
| 650                      | 74.8                                                 | 72.5 | 71.4 | 70.3 | 68.7 | 67.6 | 66.6 | 65.6 | 65.1 | 64.6 | 63.7 |

**TABLE 2.12** Reduction of the Barometer to Sea Level—Metric Units (*Continued*)

| Altitude<br>in<br>Meters | Mean Temperature of Air Column in Centigrade Degrees |       |       |       |       |       |       |       |       |       |       |
|--------------------------|------------------------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|                          | − 16°                                                | − 8°  | − 4°  | 0°    | 6°    | 10°   | 14°   | 18°   | 20°   | 22°   | 26°   |
| 700                      | 80.6                                                 | 78.1  | 76.9  | 75.7  | 74.0  | 72.9  | 71.7  | 70.7  | 70.1  | 69.6  | 68.6  |
| 750                      | 86.3                                                 | 83.7  | 82.4  | 81.1  | 79.3  | 78.1  | 76.9  | 75.7  | 75.1  | 74.6  | 73.5  |
| 800                      | 92.1                                                 | 89.2  | 87.9  | 86.5  | 84.6  | 83.3  | 82.0  | 80.8  | 80.1  | 79.6  | 78.4  |
| 850                      | 97.8                                                 | 94.8  | 93.4  | 92.0  | 89.8  | 88.5  | 87.1  | 85.8  | 85.2  | 84.5  | 83.3  |
| 900                      | 103.6                                                | 100.4 | 98.9  | 97.4  | 95.1  | 93.7  | 92.2  | 90.8  | 90.2  | 89.5  | 88.2  |
| 950                      | 109.3                                                | 106.0 | 104.4 | 102.8 | 100.4 | 98.9  | 97.4  | 95.9  | 95.2  | 94.5  | 93.1  |
| 1000                     | 115.1                                                | 111.5 | 109.8 | 108.2 | 105.7 | 104.1 | 102.5 | 100.9 | 100.2 | 99.4  | 98.0  |
| 1050                     | 120.8                                                | 117.1 | 115.3 | 113.6 | 111.0 | 109.3 | 107.6 | 106.0 | 105.2 | 104.4 | 102.9 |
| 1100                     | 126.6                                                | 122.7 | 120.8 | 119.0 | 116.3 | 114.5 | 112.7 | 111.0 | 110.2 | 109.4 | 107.8 |
| 1150                     | 132.3                                                | 128.3 | 126.3 | 124.4 | 121.6 | 119.7 | 117.9 | 116.1 | 115.2 | 114.4 | 112.7 |
| 1200                     | 138.1                                                | 133.8 | 131.8 | 129.8 | 126.8 | 124.9 | 123.0 | 121.1 | 120.2 | 119.3 | 117.6 |
| 1250                     | 143.8                                                | 139.4 | 137.3 | 135.2 | 132.1 | 130.1 | 128.1 | 126.2 | 125.2 | 124.3 | 122.5 |
| 1300                     | 149.6                                                | 145.0 | 142.8 | 140.6 | 137.4 | 135.3 | 133.2 | 131.2 | 130.2 | 129.3 | 127.4 |
| 1350                     | 155.3                                                | 150.6 | 148.3 | 146.0 | 142.7 | 140.5 | 138.4 | 136.3 | 135.2 | 134.2 | 132.3 |
| 1400                     | 161.1                                                | 156.2 | 153.8 | 151.4 | 148.0 | 145.7 | 143.5 | 141.3 | 140.2 | 139.2 | 137.2 |
| 1450                     | 166.8                                                | 161.7 | 159.3 | 156.8 | 153.3 | 150.9 | 148.6 | 146.4 | 145.3 | 144.2 | 142.1 |
| 1500                     | 172.6                                                | 167.3 | 164.8 | 162.3 | 158.5 | 156.1 | 153.7 | 151.4 | 150.3 | 149.1 | 147.0 |
| 1550                     | 178.3                                                | 172.9 | 170.2 | 167.7 | 163.8 | 161.3 | 158.8 | 156.4 | 155.3 | 154.1 | 151.8 |
| 1600                     | 184.1                                                | 178.5 | 175.7 | 173.1 | 169.1 | 166.5 | 164.0 | 161.5 | 160.3 | 159.1 | 156.7 |
| 1650                     | 189.8                                                | 184.0 | 181.2 | 178.5 | 174.4 | 171.7 | 169.1 | 166.5 | 165.3 | 164.1 | 161.6 |
| 1700                     | 195.6                                                | 189.6 | 186.7 | 183.9 | 179.7 | 176.9 | 174.2 | 171.6 | 170.3 | 169.0 | 166.5 |
| 1750                     | 201.4                                                | 195.2 | 192.2 | 189.3 | 185.0 | 182.1 | 179.3 | 176.6 | 175.3 | 174.0 | 171.4 |
| 1800                     | 207.1                                                | 200.8 | 197.7 | 194.7 | 190.2 | 187.3 | 184.5 | 181.7 | 180.3 | 179.0 | 176.3 |
| 1850                     | 212.9                                                | 206.3 | 203.2 | 200.1 | 195.5 | 192.5 | 189.6 | 186.7 | 185.3 | 183.9 | 181.2 |
| 1900                     | 218.6                                                | 211.9 | 208.7 | 205.5 | 200.8 | 197.7 | 194.7 | 191.8 | 190.3 | 188.9 | 186.1 |
| 1950                     | 224.4                                                | 217.5 | 214.2 | 210.9 | 206.1 | 202.9 | 199.8 | 196.8 | 195.3 | 193.9 | 191.0 |
| 2000                     | 230.1                                                | 223.0 | 219.7 | 216.3 | 211.4 | 208.1 | 204.9 | 201.9 | 200.3 | 198.8 | 195.0 |
| 2050                     | 235.9                                                | 228.6 | 225.1 | 221.7 | 216.7 | 213.3 | 210.1 | 206.9 | 205.3 | 203.8 | 200.8 |
| 2100                     | 241.6                                                | 234.2 | 230.6 | 227.1 | 221.9 | 218.5 | 215.2 | 211.9 | 210.4 | 208.8 | 205.7 |
| 2150                     | 247.4                                                | 239.8 | 236.1 | 232.5 | 227.2 | 223.7 | 220.3 | 217.0 | 215.4 | 213.8 | 210.6 |
| 2200                     | 253.1                                                | 245.4 | 241.6 | 237.9 | 232.5 | 228.9 | 225.4 | 222.0 | 220.4 | 218.7 | 215.5 |
| 2250                     | 258.9                                                | 250.9 | 247.1 | 243.4 | 237.8 | 234.1 | 230.6 | 227.1 | 225.4 | 223.7 | 220.4 |
| 2300                     | 264.6                                                | 256.5 | 252.6 | 248.8 | 243.1 | 239.3 | 235.7 | 232.1 | 230.4 | 228.7 | 225.3 |
| 2350                     | 270.4                                                | 262.1 | 258.1 | 254.2 | 248.3 | 244.5 | 240.8 | 237.2 | 235.4 | 233.6 | 230.2 |
| 2400                     | 276.1                                                | 267.7 | 263.6 | 259.6 | 253.6 | 249.7 | 245.9 | 242.2 | 240.4 | 238.6 | 235.1 |
| 2450                     | 281.9                                                | 273.2 | 269.1 | 265.0 | 258.9 | 254.9 | 251.0 | 247.3 | 245.4 | 243.6 | 240.0 |
| 2500                     | 287.6                                                | 278.8 | 274.5 | 270.4 | 264.2 | 260.1 | 256.2 | 252.3 | 250.4 | 248.5 | 244.9 |
| 2550                     | 293.4                                                | 284.4 | 280.0 | 275.8 | 269.5 | 265.3 | 261.3 | 257.3 | 255.4 | 253.5 | 249.8 |
| 2600                     | 299.1                                                | 290.0 | 285.5 | 281.2 | 274.8 | 270.5 | 266.4 | 262.4 | 260.4 | 258.5 | 254.7 |
| 2650                     | 304.9                                                | 295.5 | 291.0 | 286.6 | 280.0 | 275.7 | 271.5 | 267.4 | 265.4 | 263.4 | 259.6 |
| 2700                     | 310.6                                                | 301.1 | 296.5 | 292.0 | 285.3 | 280.9 | 276.6 | 272.5 | 270.4 | 268.4 | 264.5 |
| 2750                     | 316.4                                                | 306.7 | 302.0 | 297.4 | 290.6 | 286.1 | 281.8 | 277.5 | 275.4 | 273.4 | 269.4 |
| 2800                     | 322.1                                                | 312.3 | 307.5 | 302.8 | 295.9 | 291.3 | 286.9 | 282.6 | 280.4 | 278.3 | 274.3 |
| 2850                     | 327.9                                                | 317.8 | 313.0 | 308.2 | 301.2 | 296.5 | 292.0 | 287.6 | 285.4 | 283.3 | 279.2 |
| 2900                     | 333.6                                                | 323.4 | 318.4 | 313.6 | 306.4 | 301.7 | 297.1 | 292.6 | 290.4 | 288.3 | 284.1 |
| 2950                     | 339.4                                                | 329.0 | 323.9 | 319.0 | 311.7 | 306.9 | 302.2 | 297.7 | 295.5 | 293.3 | 289.0 |
| 3000                     | 345.1                                                | 334.5 | 329.4 | 324.4 | 317.0 | 312.1 | 307.4 | 302.7 | 300.5 | 298.2 | 293.8 |

\* From *Smithsonian Meteorological Tables*, 3d ed., 1907.

**TABLE 2.12** Reduction of the Barometer to Sea Level—Metric Units (*Continued*)

*B. Values in millimeters to be added.\**

| Temp.<br>—Alt.<br>Factor | Barometer Reading in Millimeters |       |       |       |       |       |      |
|--------------------------|----------------------------------|-------|-------|-------|-------|-------|------|
|                          | 790                              | 770   | 750   | 730   | 710   | 690   | 670  |
| 1                        | 0.9                              | 0.9   | 0.9   | 0.8   | 0.8   | 0.8   |      |
| 5                        | 4.6                              | 4.4   | 4.3   | 4.2   | 4.1   | 4.0   |      |
| 10                       | 9.1                              | 8.9   | 8.7   | 8.5   | 8.2   | 8.0   |      |
| 15                       | 13.8                             | 13.4  | 13.1  | 12.7  | 12.4  | 12.0  |      |
| 20                       | 18.4                             | 17.9  | 17.5  | 17.0  | 16.5  | 16.1  |      |
| 25                       |                                  | 22.5  | 21.9  | 21.3  | 20.7  | 20.1  |      |
| 30                       |                                  | 27.1  | 26.4  | 25.7  | 25.0  | 24.2  |      |
| 35                       |                                  | 31.7  | 30.8  | 30.0  | 29.2  | 28.4  |      |
| 40                       |                                  | 36.3  | 35.3  | 34.4  | 33.5  | 32.5  | 31.6 |
| 45                       |                                  |       | 39.9  | 38.8  | 37.8  | 36.7  | 35.6 |
|                          | 750                              | 730   | 710   | 690   | 670   | 650   | 630  |
| 50                       | 44.4                             | 43.3  | 42.1  | 40.9  | 39.7  |       |      |
| 55                       | 49.0                             | 47.7  | 46.4  | 45.1  | 43.8  |       |      |
| 60                       | 53.6                             | 52.2  | 50.8  | 49.3  | 47.9  |       |      |
| 65                       | 58.3                             | 56.7  | 55.2  | 53.6  | 52.1  |       |      |
| 70                       |                                  | 61.3  | 59.6  | 57.9  | 56.2  |       |      |
| 75                       |                                  | 65.8  | 64.0  | 62.2  | 60.4  |       |      |
| 80                       |                                  | 70.4  | 68.5  | 66.6  | 64.6  | 62.7  | 60.8 |
| 85                       |                                  | 75.0  | 73.0  | 70.9  | 68.9  | 66.8  | 64.8 |
| 90                       |                                  |       | 77.5  | 75.3  | 73.1  | 71.0  | 68.8 |
| 95                       |                                  |       | 82.1  | 79.7  | 77.4  | 75.1  | 72.8 |
|                          | 710                              | 690   | 670   | 650   | 630   | 610   |      |
| 100                      | 86.6                             | 84.2  | 81.8  | 79.3  | 76.9  |       |      |
| 105                      | 91.2                             | 88.7  | 86.1  | 83.5  | 81.0  |       |      |
| 110                      | 95.9                             | 93.2  | 90.5  | 87.8  | 85.1  |       |      |
| 115                      | 100.5                            | 97.7  | 94.8  | 92.0  | 89.2  |       |      |
| 120                      |                                  | 102.2 | 99.3  | 96.3  | 93.3  |       |      |
| 125                      |                                  | 106.8 | 103.7 | 100.6 | 97.5  | 94.4  |      |
| 130                      |                                  | 111.4 | 108.2 | 104.9 | 101.7 | 98.5  |      |
| 135                      |                                  | 116.0 | 112.7 | 109.3 | 105.9 | 102.6 |      |
| 140                      |                                  | 120.7 | 117.2 | 113.7 | 110.2 | 106.7 |      |
| 145                      |                                  |       | 121.7 | 118.1 | 114.5 | 110.8 |      |
|                          | 670                              | 650   | 630   | 610   | 590   | 570   |      |
| 150                      | 126.3                            | 122.5 | 118.8 | 115.0 |       |       |      |
| 155                      | 130.9                            | 127.0 | 123.1 | 119.2 |       |       |      |
| 160                      | 135.5                            | 131.5 | 127.4 | 123.4 |       |       |      |
| 165                      | 140.2                            | 136.0 | 131.8 | 127.6 |       |       |      |
| 170                      |                                  | 140.5 | 136.2 | 131.9 | 127.5 | 123.2 |      |
| 175                      |                                  | 145.1 | 140.6 | 136.2 | 131.7 | 127.2 |      |
| 180                      |                                  | 149.7 | 145.1 | 140.5 | 135.9 | 131.3 |      |
| 185                      |                                  | 154.3 | 149.5 | 144.8 | 140.0 | 135.3 |      |
| 190                      |                                  | 158.9 | 154.0 | 149.2 | 144.3 | 139.4 |      |
| 195                      |                                  |       | 158.6 | 153.5 | 148.5 | 143.5 |      |

\* From *Smithsonian Meteorological Tables*, 3d ed., 1907.



**TABLE 2.12** Reduction of the Barometer to Sea Level—Metric Units (*Continued*)

*B. Values in millimeters to be added.\**

| Temp.<br>—Alt.<br>Factor | Barometer Reading in Millimeters |       |       |       |       |       |
|--------------------------|----------------------------------|-------|-------|-------|-------|-------|
|                          | 630                              | 610   | 590   | 570   | 550   | 530   |
| 200                      | 163.1                            | 157.9 | 152.8 | 147.6 |       |       |
| 205                      | 167.7                            | 162.4 | 157.1 | 151.7 |       |       |
| 210                      | 172.3                            | 166.8 | 161.4 | 155.9 |       |       |
| 215                      | 176.9                            | 171.3 | 165.7 | 160.1 | 154.5 | 148.9 |
| 220                      |                                  | 175.8 | 170.1 | 164.3 | 158.5 | 152.8 |
| 225                      |                                  | 180.4 | 174.5 | 168.5 | 162.6 | 156.7 |
| 230                      |                                  | 184.9 | 178.9 | 172.8 | 166.7 | 160.7 |
| 235                      |                                  | 189.5 | 183.3 | 177.1 | 170.9 | 164.7 |
| 240                      |                                  | 194.1 | 187.8 | 181.4 | 175.0 | 168.7 |
| 245                      |                                  | 198.8 | 192.3 | 185.7 | 179.2 | 172.7 |
|                          | 590                              | 570   | 550   | 530   | 510   |       |
| 250                      | 196.8                            | 190.1 | 183.4 | 176.8 |       |       |
| 255                      | 201.3                            | 194.5 | 187.7 | 180.8 |       |       |
| 260                      | 205.9                            | 198.9 | 191.9 | 185.0 | 178.0 |       |
| 265                      | 210.5                            | 203.3 | 196.2 | 189.1 | 181.9 |       |
| 270                      | 215.1                            | 207.8 | 200.5 | 193.2 | 185.9 |       |
| 275                      | 219.8                            | 212.3 | 204.9 | 197.4 | 190.0 |       |
| 280                      |                                  | 216.8 | 209.2 | 201.6 | 194.0 |       |
| 285                      |                                  | 221.4 | 213.6 | 205.8 | 198.1 |       |
| 290                      |                                  | 225.9 | 218.0 | 210.1 | 202.1 |       |
| 295                      |                                  | 230.5 | 222.4 | 214.3 | 206.3 |       |
|                          | 570                              | 550   | 530   | 510   | 490   |       |
| 300                      | 235.1                            | 226.9 | 218.6 | 210.4 |       |       |
| 305                      | 239.8                            | 231.4 | 223.0 | 214.6 | 206.1 |       |
| 310                      |                                  | 235.9 | 227.3 | 218.7 | 210.1 |       |
| 315                      |                                  | 240.4 | 231.7 | 222.9 | 214.2 |       |
| 320                      |                                  | 245.0 | 236.1 | 227.2 | 218.3 |       |
| 325                      |                                  | 249.6 | 240.5 | 231.4 | 222.4 |       |
| 330                      |                                  | 254.2 | 244.9 | 235.7 | 226.5 |       |
| 335                      |                                  | 258.8 | 249.4 | 240.0 | 230.6 |       |
| 340                      |                                  | 263.5 | 253.9 | 244.4 | 234.8 |       |
| 345                      |                                  |       | 258.4 | 248.7 | 238.9 |       |

\* From *Smithsonian Meteorological Tables*, 3d ed., 1907.

**TABLE 2.13** Viscosity Conversion Table  
*Centistokes to Saybolt, Redwood, and Engler units.*

Poise = cgs unit of absolute viscosity      Centipoise = 0.01 poise

Stoke = cgs unit of kinematic viscosity      Centistoke = 0.01 stoke

Centipoises = centistokes × density (at temperature under consideration)

Reyn (1 lb · s per sq in) = 69 × 10<sup>5</sup> centipoises

Cf. *Jour. Inst. Pet. Tech.*, Vol. 22, p. 21 (1936); *Reports of A. S. T. M. Committee D-2, 1936 and 1937.*  
The values of Saybolt Universal Viscosity at 100°F and at 210°F are taken directly from the comprehensive *ASTM Viscosity Table, Special Technical Publication No. 43A* (1953) by permission of the publishers, American Society for Testing Materials, 1916 Race St., Philadelphia 3, Pa.

| Centistokes | Saybolt Universal Viscosity at |        |        | Redwood Seconds at |        |        | Engler<br>Degrees at<br>all Temps. |
|-------------|--------------------------------|--------|--------|--------------------|--------|--------|------------------------------------|
|             | 100°F.                         | 130°F. | 210°F. | 70°F.              | 140°F. | 200°F. |                                    |
| 2.0         | 32.62                          | 32.68  | 32.85  | 30.2               | 31.0   | 31.2   | 1.14                               |
| 3.0         | 36.03                          | 36.10  | 36.28  | 32.7               | 33.5   | 33.7   | 1.22                               |
| 4.0         | 39.14                          | 39.22  | 39.41  | 35.3               | 36.0   | 36.3   | 1.31                               |
| 5.0         | 42.35                          | 42.43  | 42.65  | 37.9               | 38.5   | 38.9   | 1.40                               |
| 6.0         | 45.56                          | 45.65  | 45.88  | 40.5               | 41.0   | 41.5   | 1.48                               |
| 7.0         | 48.77                          | 48.86  | 49.11  | 43.2               | 43.7   | 44.2   | 1.56                               |
| 8.0         | 52.09                          | 52.19  | 52.45  | 46.0               | 46.4   | 46.9   | 1.65                               |
| 9.0         | 55.50                          | 55.61  | 55.89  | 48.9               | 49.1   | 49.7   | 1.75                               |
| 10.0        | 58.91                          | 59.02  | 59.32  | 51.7               | 52.0   | 52.6   | 1.84                               |
| 11.0        | 62.43                          | 62.55  | 62.86  | 54.8               | 55.0   | 55.6   | 1.93                               |
| 12.0        | 66.04                          | 66.17  | 66.50  | 57.9               | 58.1   | 58.8   | 2.02                               |
| 14.0        | 73.57                          | 73.71  | 74.09  | 64.4               | 64.6   | 65.3   | 2.22                               |
| 16.0        | 81.30                          | 81.46  | 81.87  | 71.0               | 71.4   | 72.2   | 2.43                               |
| 18.0        | 89.44                          | 89.61  | 90.06  | 77.9               | 78.5   | 79.4   | 2.64                               |
| 20.0        | 97.77                          | 97.96  | 98.45  | 85.0               | 85.8   | 86.9   | 2.87                               |
| 22.0        | 106.4                          | 106.6  | 107.1  | 92.4               | 93.3   | 94.5   | 3.10                               |
| 24.0        | 115.0                          | 115.2  | 115.8  | 99.9               | 100.9  | 102.2  | 3.34                               |
| 26.0        | 123.7                          | 123.9  | 124.5  | 107.5              | 108.6  | 110.0  | 3.58                               |
| 28.0        | 132.5                          | 132.8  | 133.4  | 115.3              | 116.5  | 118.0  | 3.82                               |
| 30.0        | 141.3                          | 141.6  | 142.3  | 123.1              | 124.4  | 126.0  | 4.07                               |
| 32.0        | 150.2                          | 150.5  | 151.2  | 131.0              | 132.3  | 134.1  | 4.32                               |
| 34.0        | 159.2                          | 159.5  | 160.3  | 138.9              | 140.2  | 142.2  | 4.57                               |
| 36.0        | 168.2                          | 168.5  | 169.4  | 146.9              | 148.2  | 150.3  | 4.83                               |
| 38.0        | 177.3                          | 177.6  | 178.5  | 155.0              | 156.2  | 158.3  | 5.08                               |
| 40.0        | 186.3                          | 186.7  | 187.6  | 163.0              | 164.3  | 166.7  | 5.34                               |
| 42.0        | 195.3                          | 195.7  | 196.7  | 171.0              | 172.3  | 175.0  | 5.59                               |
| 44.0        | 204.4                          | 204.8  | 205.9  | 179.1              | 180.4  | 183.3  | 5.85                               |
| 46.0        | 213.7                          | 214.1  | 215.2  | 187.1              | 188.5  | 191.7  | 6.11                               |
| 48.0        | 222.9                          | 223.3  | 224.5  | 195.2              | 196.6  | 200.0  | 6.37                               |
| 50.0        | 232.1                          | 232.5  | 233.8  | 203.3              | 204.7  | 208.3  | 6.63                               |
| 60.0        | 278.3                          | 278.8  | 280.2  | 243.5              | 245.3  | 250.0  | 7.90                               |
| 70.0        | 324.4                          | 325.0  | 326.7  | 283.9              | 286.0  | 291.7  | 9.21                               |
| 80.0        | 370.8                          | 371.5  | 373.4  | 323.9              | 326.6  | 333.4  | 10.53                              |
| 90.0        | 417.1                          | 417.9  | 420.0  | 364.4              | 367.4  | 375.0  | 11.84                              |
| 100.0*      | 463.5                          | 464.4  | 466.7  | 404.9              | 408.2  | 416.7  | 13.16                              |

\* At higher values use the same ratio as above for 100 centistokes; **e.g.**, 102 centistokes = 102 × 4.635 Saybolt seconds at 100°F.  
To obtain the Saybolt Universal viscosity equivalent to a kinematic viscosity determined at *t*°F., multiply the equivalent Saybolt Universal viscosity at 100°F. by 1 + (t – 100) 0.000064; **e.g.**, 10 centistokes at 210°F are equivalent to 58.91 × 1.0070, or 59.32 Saybolt Universal Viscosity at 210°F.

**TABLE 2.14** Conversion of Weighings in Air to Weighings in Vacuo

If the mass of a substance in air is  $m_f$ , its density  $\rho_m$ , the density of weights used in making the weighing  $\rho_w$ , and the density\* of air  $\rho_a$ , the true mass of the substance in vacuo,  $m_{vac}$ , is

$$m_{vac} = m_f + \rho_a m_f \left( \frac{1}{\rho_m} - \frac{1}{\rho_w} \right)$$

For most purposes it is sufficient to assume a density of 8.4 for brass weights, and a density of 0.0012 for air under ordinary conditions. The equation then becomes

$$m_{vac} = m_f + 0.0012 m_f \left( \frac{1}{\rho_m} - \frac{1}{8.4} \right)$$

The table which follows gives the values of  $k$  (buoyancy reduction factor), which is the correction necessary because of the buoyant effect of the air upon the object weighed; the table is computed for air with the density of 0.0012;  $m$  is the weight in grams of the object when weighed in air; weight of object reduced to “in vacuo” =  $m + km/1000$ .

| Density of<br>object weighed | Buoyancy reduction factor, $k$  |                                        |                                        |                               |
|------------------------------|---------------------------------|----------------------------------------|----------------------------------------|-------------------------------|
|                              | Brass weights,<br>density = 8.4 | Pt or Pt-Ir<br>weights, density = 21.5 | Al or quartz weights,<br>density = 2.7 | Gold weights,<br>density = 17 |
| 0.2                          | 5.89                            | 5.98                                   | 5.58                                   | 5.97                          |
| 0.3                          | 3.87                            | 3.96                                   | 3.56                                   | 3.95                          |
| 0.4                          | 2.87                            | 2.95                                   | 2.55                                   | 2.94                          |
| 0.5                          | 2.26                            | 2.35                                   | 1.95                                   | 2.34                          |
| 0.6                          | 1.86                            | 1.95                                   | 1.55                                   | 1.93                          |
| 0.7                          | 1.57                            | 1.66                                   | 1.26                                   | 1.65                          |
| 0.75                         | 1.46                            | 1.55                                   | 1.15                                   | 1.53                          |
| 0.80                         | 1.36                            | 1.45                                   | 1.05                                   | 1.43                          |
| 0.82                         | 1.32                            | 1.41                                   | 1.01                                   | 1.39                          |
| 0.84                         | 1.29                            | 1.37                                   | 0.98                                   | 1.36                          |
| 0.86                         | 1.25                            | 1.34                                   | 0.94                                   | 1.33                          |
| 0.88                         | 1.22                            | 1.31                                   | 0.91                                   | 1.29                          |
| 0.90                         | 1.19                            | 1.28                                   | 0.88                                   | 1.26                          |
| 0.92                         | 1.16                            | 1.25                                   | 0.85                                   | 1.24                          |
| 0.94                         | 1.13                            | 1.22                                   | 0.82                                   | 1.21                          |
| 0.96                         | 1.11                            | 1.20                                   | 0.80                                   | 1.18                          |
| 0.98                         | 1.08                            | 1.17                                   | 0.77                                   | 1.16                          |
| 1.00                         | 1.06                            | 1.15                                   | 0.75                                   | 1.13                          |
| 1.02                         | 1.03                            | 1.12                                   | 0.72                                   | 1.11                          |
| 1.04                         | 1.01                            | 1.10                                   | 0.70                                   | 1.08                          |
| 1.06                         | 0.99                            | 1.08                                   | 0.68                                   | 1.06                          |
| 1.08                         | 0.97                            | 1.06                                   | 0.66                                   | 1.04                          |
| 1.10                         | 0.95                            | 1.04                                   | 0.64                                   | 1.02                          |
| 1.12                         | 0.93                            | 1.02                                   | 0.62                                   | 1.00                          |
| 1.14                         | 0.91                            | 1.00                                   | 0.60                                   | 0.98                          |
| 1.16                         | 0.89                            | 0.98                                   | 0.58                                   | 0.96                          |
| 1.18                         | 0.87                            | 0.96                                   | 0.56                                   | 0.95                          |
| 1.20                         | 0.86                            | 0.95                                   | 0.55                                   | 0.93                          |
| 1.25                         | 0.82                            | 0.91                                   | 0.51                                   | 0.89                          |
| 1.30                         | 0.78                            | 0.87                                   | 0.47                                   | 0.85                          |

\* See Table 5.15, Specific Gravity of Air at Various Temperatures.

**TABLE 2.14** Conversion of Weighings in Air to Weighings in Vacuo (*Continued*)

| Density of<br>object weighed | Buoyancy reduction factor, <i>k</i> |                                        |                                        |                               |
|------------------------------|-------------------------------------|----------------------------------------|----------------------------------------|-------------------------------|
|                              | Brass weights,<br>density = 8.4     | Pt or Pt-Ir<br>weights, density = 21.5 | Al or quartz weights,<br>density = 2.7 | Gold weights,<br>density = 17 |
| 1.35                         | 0.75                                | 0.83                                   | 0.44                                   | 0.82                          |
| 1.40                         | 0.71                                | 0.80                                   | 0.40                                   | 0.79                          |
| 1.50                         | 0.66                                | 0.74                                   | 0.35                                   | 0.73                          |
| 1.6                          | 0.61                                | 0.69                                   | 0.30                                   | 0.68                          |
| 1.7                          | 0.56                                | 0.65                                   | 0.25                                   | 0.64                          |
| 1.8                          | 0.52                                | 0.61                                   | 0.21                                   | 0.60                          |
| 1.9                          | 0.49                                | 0.58                                   | 0.18                                   | 0.56                          |
| 2.0                          | 0.46                                | 0.54                                   | 0.15                                   | 0.53                          |
| 2.2                          | 0.40                                | 0.49                                   | 0.09                                   | 0.48                          |
| 2.4                          | 0.36                                | 0.44                                   | 0.05                                   | 0.43                          |
| 2.6                          | 0.32                                | 0.41                                   | 0.01                                   | 0.39                          |
| 2.8                          | 0.29                                | 0.37                                   | −0.02                                  | 0.36                          |
| 3.0                          | 0.26                                | 0.34                                   | −0.05                                  | 0.33                          |
| 3.5                          | 0.20                                | 0.29                                   | −0.11                                  | 0.27                          |
| 4                            | 0.16                                | 0.24                                   | −0.15                                  | 0.23                          |
| 5                            | 0.10                                | 0.18                                   | −0.21                                  | 0.17                          |
| 6                            | 0.06                                | 0.14                                   | −0.25                                  | 0.13                          |
| 7                            | 0.03                                | 0.12                                   | −0.28                                  | 0.10                          |
| 8                            | 0.01                                | 0.09                                   | −0.30                                  | 0.08                          |
| 9                            | −0.01                               | 0.08                                   | −0.32                                  | 0.06                          |
| 10                           | −0.02                               | 0.06                                   | −0.33                                  | 0.05                          |
| 12                           | −0.04                               | 0.04                                   | −0.35                                  | 0.03                          |
| 14                           | −0.06                               | 0.03                                   | −0.37                                  | 0.02                          |
| 16                           | −0.07                               | 0.02                                   | −0.38                                  | 0.00                          |
| 18                           | −0.08                               | 0.01                                   | −0.39                                  | 0.00                          |
| 20                           | −0.08                               | 0.00                                   | −0.39                                  | −0.01                         |
| 22                           | −0.09                               | 0.00                                   | −0.40                                  | −0.02                         |

TABLE 2.15 Hydrometer Conversion Table

This table gives the relation between density (c.g.s.) and degrees on the Baumé and Twaddell scales. The Twaddell scale is never used for densities less than unity. See also Sec. 2.1.2.1, Hydrometers.

| Density | Degrees Baumé<br>(NIST* scale) | Degrees Baumé<br>(A.P.I.† scale) | Density                      | Degrees Baumé<br>(NIST* scale) | Degrees Baumé<br>(A.P.I.† scale) |
|---------|--------------------------------|----------------------------------|------------------------------|--------------------------------|----------------------------------|
| 0.600   | 103.33                         | 104.33                           | 0.825                        | 39.70                          | 40.02                            |
| 0.605   | 101.40                         | 102.38                           | 0.830                        | 38.68                          | 38.98                            |
| 0.610   | 99.51                          | 100.47                           | 0.835                        | 37.66                          | 37.96                            |
| 0.615   | 97.64                          | 98.58                            | 0.840                        | 36.67                          | 36.95                            |
| 0.620   | 95.81                          | 96.73                            | 0.845                        | 35.68                          | 35.96                            |
| 0.625   | 94.00                          | 94.90                            | 0.850                        | 34.71                          | 34.97                            |
| 0.630   | 92.22                          | 93.10                            | 0.855                        | 33.74                          | 34.00                            |
| 0.635   | 90.47                          | 91.33                            | 0.860                        | 32.79                          | 33.03                            |
| 0.640   | 88.75                          | 89.59                            | 0.865                        | 31.85                          | 32.08                            |
| 0.645   | 87.05                          | 87.88                            | 0.870                        | 30.92                          | 31.14                            |
| 0.650   | 85.38                          | 86.19                            | 0.875                        | 30.00                          | 30.21                            |
| 0.655   | 83.74                          | 84.53                            | 0.880                        | 29.09                          | 29.30                            |
| 0.660   | 82.12                          | 82.89                            | 0.885                        | 28.19                          | 28.39                            |
| 0.665   | 80.52                          | 81.28                            | 0.890                        | 27.30                          | 27.49                            |
| 0.670   | 78.95                          | 79.69                            | 0.895                        | 26.42                          | 26.60                            |
| 0.675   | 77.41                          | 78.13                            | 0.900                        | 25.56                          | 25.72                            |
| 0.680   | 75.88                          | 76.59                            | 0.905                        | 24.70                          | 24.85                            |
| 0.685   | 74.38                          | 75.07                            | 0.910                        | 23.85                          | 23.99                            |
| 0.690   | 72.90                          | 73.57                            | 0.915                        | 23.01                          | 23.14                            |
| 0.695   | 71.43                          | 72.10                            | 0.920                        | 22.17                          | 22.30                            |
| 0.700   | 70.00                          | 70.64                            | 0.925                        | 21.35                          | 21.47                            |
| 0.705   | 68.57                          | 69.21                            | 0.930                        | 20.54                          | 20.65                            |
| 0.710   | 67.18                          | 67.80                            | 0.935                        | 19.73                          | 19.84                            |
| 0.715   | 65.80                          | 66.40                            | 0.940                        | 18.94                          | 19.03                            |
| 0.720   | 64.44                          | 65.03                            | 0.945                        | 18.15                          | 18.24                            |
| 0.725   | 63.10                          | 63.67                            | 0.950                        | 17.37                          | 17.45                            |
| 0.730   | 61.78                          | 62.34                            | 0.955                        | 16.60                          | 16.67                            |
| 0.735   | 60.48                          | 61.02                            | 0.960                        | 15.83                          | 15.90                            |
| 0.740   | 59.19                          | 59.72                            | 0.965                        | 15.08                          | 15.13                            |
| 0.745   | 57.92                          | 58.43                            | 0.970                        | 14.33                          | 14.38                            |
| 0.750   | 56.67                          | 57.17                            | 0.975                        | 13.59                          | 13.63                            |
| 0.755   | 55.43                          | 55.92                            | 0.980                        | 12.86                          | 12.89                            |
| 0.760   | 54.21                          | 54.68                            | 0.985                        | 12.13                          | 12.15                            |
| 0.765   | 53.01                          | 53.47                            | 0.990                        | 11.41                          | 11.43                            |
| 0.770   | 51.82                          | 52.27                            | 0.995                        | 10.70                          | 10.71                            |
| 0.775   | 50.65                          | 51.08                            | 1.000                        | 10.00                          | 10.00                            |
| 0.780   | 49.49                          | 49.91                            | DENSITIES GREATER THAN UNITY |                                |                                  |
| 0.785   | 48.34                          | 48.75                            | Density                      | Degrees Baumé<br>(NIST* scale) | Degrees Twaddell                 |
| 0.790   | 47.22                          | 47.61                            | 1.00                         | 0.00                           | 0                                |
| 0.795   | 46.10                          | 46.49                            | 1.01                         | 1.44                           | 2                                |
| 0.800   | 45.00                          | 45.38                            | 1.02                         | 2.84                           | 4                                |
| 0.805   | 43.91                          | 44.28                            |                              |                                |                                  |
| 0.810   | 42.84                          | 43.19                            |                              |                                |                                  |
| 0.815   | 41.78                          | 42.12                            |                              |                                |                                  |
| 0.820   | 40.73                          | 41.06                            |                              |                                |                                  |

\* NIST, National Institute for Science and Technology (formerly the National Bureau of Standards, U.S.).  
† A.P.I. is the American Petroleum Institute.

**TABLE 2.15** Hydrometer Conversion Table (*Continued*)

| Density | Degrees Baumé<br>(NIST* scale) | Degrees<br>Twaddell | Density | Degrees Baumé<br>(NIST* scale) | Degrees<br>Twaddell |
|---------|--------------------------------|---------------------|---------|--------------------------------|---------------------|
| 1.03    | 4.22                           | 6                   | 1.52    | 49.60                          | 104                 |
| 1.04    | 5.58                           | 8                   | 1.53    | 50.23                          | 106                 |
| 1.05    | 6.91                           | 10                  | 1.54    | 50.84                          | 108                 |
| 1.06    | 8.21                           | 12                  | 1.55    | 51.45                          | 110                 |
| 1.07    | 9.49                           | 14                  | 1.56    | 52.05                          | 112                 |
| 1.08    | 10.78                          | 16                  | 1.57    | 52.64                          | 114                 |
| 1.09    | 11.97                          | 18                  | 1.58    | 53.23                          | 116                 |
| 1.10    | 13.18                          | 20                  | 1.59    | 53.80                          | 118                 |
| 1.11    | 14.37                          | 22                  | 1.60    | 54.38                          | 120                 |
| 1.12    | 15.54                          | 24                  | 1.61    | 54.94                          | 122                 |
| 1.13    | 16.68                          | 26                  | 1.62    | 55.49                          | 124                 |
| 1.14    | 17.81                          | 28                  | 1.63    | 56.04                          | 126                 |
| 1.15    | 18.91                          | 30                  | 1.64    | 56.58                          | 128                 |
| 1.16    | 20.00                          | 32                  | 1.65    | 57.12                          | 130                 |
| 1.17    | 21.07                          | 34                  | 1.66    | 57.65                          | 132                 |
| 1.18    | 22.12                          | 36                  | 1.67    | 58.17                          | 134                 |
| 1.19    | 23.15                          | 38                  | 1.68    | 58.69                          | 136                 |
| 1.20    | 24.17                          | 40                  | 1.69    | 59.20                          | 138                 |
| 1.21    | 25.16                          | 42                  | 1.70    | 59.71                          | 140                 |
| 1.22    | 26.15                          | 44                  | 1.71    | 60.20                          | 142                 |
| 1.23    | 27.11                          | 46                  | 1.72    | 60.70                          | 144                 |
| 1.24    | 28.06                          | 48                  | 1.73    | 61.18                          | 146                 |
| 1.25    | 29.00                          | 50                  | 1.74    | 61.67                          | 148                 |
| 1.26    | 29.92                          | 52                  | 1.75    | 62.14                          | 150                 |
| 1.27    | 30.83                          | 54                  | 1.76    | 62.61                          | 152                 |
| 1.28    | 31.72                          | 56                  | 1.77    | 63.08                          | 154                 |
| 1.29    | 32.60                          | 58                  | 1.78    | 63.54                          | 156                 |
| 1.30    | 33.46                          | 60                  | 1.79    | 63.99                          | 158                 |
| 1.31    | 34.31                          | 62                  | 1.80    | 64.44                          | 160                 |
| 1.32    | 35.15                          | 64                  | 1.81    | 64.89                          | 162                 |
| 1.33    | 35.98                          | 66                  | 1.82    | 65.31                          | 164                 |
| 1.34    | 36.79                          | 68                  | 1.83    | 65.77                          | 166                 |
| 1.35    | 37.59                          | 70                  | 1.84    | 66.20                          | 168                 |
| 1.36    | 38.38                          | 72                  | 1.85    | 66.62                          | 170                 |
| 1.37    | 39.16                          | 74                  | 1.86    | 67.04                          | 172                 |
| 1.38    | 39.93                          | 76                  | 1.87    | 67.46                          | 174                 |
| 1.39    | 40.68                          | 78                  | 1.88    | 67.87                          | 176                 |
| 1.40    | 41.43                          | 80                  | 1.89    | 68.28                          | 178                 |
| 1.41    | 42.16                          | 82                  | 1.90    | 68.68                          | 180                 |
| 1.42    | 42.89                          | 84                  | 1.91    | 69.08                          | 182                 |
| 1.43    | 43.60                          | 86                  | 1.92    | 69.48                          | 184                 |
| 1.44    | 44.31                          | 88                  | 1.93    | 69.87                          | 186                 |
| 1.45    | 45.00                          | 90                  | 1.94    | 70.26                          | 188                 |
| 1.46    | 45.68                          | 92                  | 1.95    | 70.64                          | 190                 |
| 1.47    | 46.36                          | 94                  | 1.96    | 71.02                          | 192                 |
| 1.48    | 47.03                          | 96                  | 1.97    | 71.40                          | 194                 |
| 1.49    | 47.68                          | 98                  | 1.98    | 71.77                          | 196                 |
| 1.50    | 48.33                          | 100                 | 1.99    | 72.14                          | 198                 |
| 1.51    | 48.97                          | 102                 | 2.00    | 72.50                          | 200                 |

\* NIST, National Institute for Science and Tchnology (formerly the National Bureau of Standards, U.S.).

**TABLE 2.16** Pressure Conversion Chart

| psi   | Inches H <sub>2</sub> O<br>at 4°C | Inches Hg<br>at 0°C | mmH <sub>2</sub> O<br>at 4°C | mmHg<br>at 0°C | atm    | Pascals<br>(N · m <sup>-2</sup> ) |
|-------|-----------------------------------|---------------------|------------------------------|----------------|--------|-----------------------------------|
| 0.01  | 0.2768                            | 0.0204              | 7.031                        | 0.517          | 0.0007 | 68.95                             |
| 0.02  | 0.5536                            | 0.0407              | 14.06                        | 1.034          | 0.0014 | 137.90                            |
| 0.03  | 0.8304                            | 0.0611              | 21.09                        | 1.551          | 0.0020 | 206.8                             |
| 0.04  | 1.107                             | 0.0814              | 28.12                        | 2.068          | 0.0027 | 275.8                             |
| 0.05  | 1.384                             | 0.1018              | 35.15                        | 2.586          | 0.0034 | 344.7                             |
| 0.06  | 1.661                             | 0.1222              | 42.18                        | 3.103          | 0.0041 | 413.7                             |
| 0.07  | 1.938                             | 0.1425              | 49.22                        | 3.620          | 0.0048 | 482.6                             |
| 0.08  | 2.214                             | 0.1629              | 56.25                        | 4.137          | 0.0054 | 551.6                             |
| 0.09  | 2.491                             | 0.1832              | 63.28                        | 4.654          | 0.0061 | 620.5                             |
| 0.10  | 2.768                             | 0.2036              | 70.31                        | 5.171          | 0.0068 | 689.5                             |
| 0.20  | 5.536                             | 0.4072              | 140.6                        | 10.34          | 0.0136 | 1 379.9                           |
| 0.30  | 8.304                             | 0.6108              | 210.9                        | 15.51          | 0.0204 | 2 068.5                           |
| 0.40  | 11.07                             | 0.8144              | 281.2                        | 20.68          | 0.0272 | 2 758                             |
| 0.50  | 13.84                             | 1.018               | 351.5                        | 25.86          | 0.0340 | 3 447                             |
| 0.60  | 16.61                             | 1.222               | 421.8                        | 31.03          | 0.0408 | 4 137                             |
| 0.70  | 19.38                             | 1.425               | 492.2                        | 36.20          | 0.0476 | 4 826                             |
| 0.80  | 22.14                             | 1.629               | 562.5                        | 41.37          | 0.0544 | 5 516                             |
| 0.90  | 24.91                             | 1.832               | 632.8                        | 46.54          | 0.0612 | 6 205                             |
| 1.00  | 27.68                             | 2.036               | 703.1                        | 51.71          | 0.0689 | 6 895                             |
| 2.00  | 55.36                             | 4.072               | 1 072                        | 103.4          | 0.1361 | 13 790                            |
| 3.00  | 83.04                             | 6.108               | 2 109                        | 155.1          | 0.2041 | 20 684                            |
| 4.00  | 110.7                             | 8.144               | 2 812                        | 206.8          | 0.2722 | 27 579                            |
| 5.00  | 138.4                             | 10.18               | 3 515                        | 258.6          | 0.3402 | 34 474                            |
| 6.00  | 166.1                             | 12.22               | 4 218                        | 310.3          | 0.4083 | 41 369                            |
| 7.00  | 193.8                             | 14.25               | 4 922                        | 362.0          | 0.4763 | 48 263                            |
| 8.00  | 221.4                             | 16.29               | 5 625                        | 413.7          | 0.5444 | 55 158                            |
| 9.00  | 249.1                             | 18.32               | 6 328                        | 465.4          | 0.6124 | 62 053                            |
| 10.0  | 276.8                             | 20.36               | 7 031                        | 517.1          | 0.6805 | 68 948                            |
| 14.7  | 406.9                             | 29.93               | 10 332                       | 760.0          | 1.000  | 101 325                           |
| 15.0  | 415.2                             | 30.54               | 10 550                       | 775.7          | 1.021  | 103 421                           |
| 20.0  | 553.6                             | 40.72               | 14 060                       | 1 034          | 1.361  | 137 895                           |
| 25.0  | 692.0                             | 50.90               | 17 580                       | 1 293          | 1.701  | 172 369                           |
| 30.0  | 830.4                             | 61.08               | 21 090                       | 1 551          | 2.041  | 206 843                           |
| 40.0  | 1 107                             | 81.44               | 28 120                       | 2 068          | 2.722  | 275 790                           |
| 50.0  | 1 384                             | 101.8               | 35 150                       | 2 586          | 3.402  | 344 738                           |
| 60.0  | 1 661                             | 122.2               | 42 180                       | 3 103          | 4.083  | 413 685                           |
| 70.0  | 1 938                             | 142.5               | 49 220                       | 3 620          | 4.763  | 482 633                           |
| 80.0  | 2 214                             | 162.9               | 56 250                       | 4 137          | 5.444  | 551 581                           |
| 90.0  | 2 491                             | 183.2               | 63 280                       | 4 654          | 6.124  | 620 528                           |
| 100.0 | 2 768                             | 203.6               | 70 307                       | 5 171          | 6.805  | 689 476                           |
| 150.0 | 4 152                             | 305.4               |                              | 7 757          | 10.21  | 1 034 214                         |
| 200.0 | 5 536                             | 407.2               |                              | 10 343         | 13.61  | 1 378 951                         |
| 250.0 | 6 920                             | 509.0               |                              |                | 17.01  | 1 723 689                         |
| 300.0 | 8 304                             | 610.8               |                              |                | 20.41  | 2 068 427                         |
| 400.0 |                                   |                     |                              |                | 27.22  | 2 757 903                         |
| 500.0 |                                   |                     |                              |                | 34.02  | 3 447 379                         |

1 bar = 10<sup>5</sup> pascal.

TABLE 2.17 Corrections to Be Added to Molar Values to Convert to Molal

| Temperature,<br>°C | Aqueous solution                        |                                         |                                                            |                                                              |
|--------------------|-----------------------------------------|-----------------------------------------|------------------------------------------------------------|--------------------------------------------------------------|
|                    | $\Delta G^\circ$<br>J·mol <sup>-1</sup> | $\Delta H^\circ$<br>J·mol <sup>-1</sup> | $\Delta S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $\Delta C^\circ_p$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
| 0                  | 0.4                                     | −42.7                                   | −0.17                                                      | 55.2                                                         |
| 10                 | 0.8                                     | 58.1                                    | 0.21                                                       | 45.6                                                         |
| 20                 | 4.2                                     | 148.1                                   | 0.50                                                       | 38.9                                                         |
| 30                 | 10.9                                    | 230.5                                   | 0.79                                                       | 35.1                                                         |
| 40                 | 20.1                                    | 313.4                                   | 1.09                                                       | 33.0                                                         |
| 50                 | 32.2                                    | 397.9                                   | 1.34                                                       | 32.6                                                         |
| 60                 | 46.8                                    | 482.4                                   | 1.59                                                       | 32.2                                                         |

TABLE 2.18 Molar Equivalent of One Liter of Gas at Various Temperatures and Pressures

The values in this table, which give the number of moles in 1 liter of gas, are based on the properties of an “ideal” gas and were calculated by use of the formula:

Moles/liter =  $\frac{P}{760} \times \frac{273}{T} \times \frac{1}{22.40}$

where *P* is the pressure in millimeters of mercury and *T* is the temperature in kelvins (= *t*°C + 273).  
To convert to moles per cubic foot multiply the values in the table by 28.316.

| Pressure<br>mm of<br>mercury | Temperature °C |         |         |         |         |         |
|------------------------------|----------------|---------|---------|---------|---------|---------|
|                              | 10°            | 12°     | 14°     | 16°     | 18°     | 20°     |
| 655                          | 0.03712        | 0.03686 | 0.03660 | 0.03634 | 0.03610 | 0.03585 |
| 660                          | 3731           | 3714    | 3688    | 3662    | 3637    | 3612    |
| 665                          | 3768           | 3742    | 3716    | 3690    | 3665    | 3640    |
| 670                          | 3796           | 3770    | 3744    | 3718    | 3692    | 3667    |
| 675                          | 3825           | 3798    | 3772    | 3745    | 3720    | 3695    |
| 680                          | 0.03853        | 0.03826 | 0.03800 | 0.03773 | 0.03747 | 0.03694 |
| 685                          | 3881           | 3854    | 3827    | 3801    | 3775    | 3749    |
| 690                          | 3910           | 3882    | 3855    | 3829    | 3802    | 3776    |
| 695                          | 3938           | 3910    | 3883    | 3856    | 3830    | 3804    |
| 700                          | 3967           | 3939    | 3911    | 3884    | 3858    | 3831    |
| 702                          | 0.03978        | 0.03950 | 0.03922 | 0.03895 | 0.03869 | 0.03842 |
| 704                          | 3989           | 3961    | 3934    | 3906    | 3880    | 3853    |
| 706                          | 4000           | 3972    | 3945    | 3917    | 3891    | 3864    |
| 708                          | 4012           | 3984    | 3956    | 3929    | 3902    | 3875    |
| 710                          | 4023           | 3995    | 3967    | 3940    | 3913    | 3886    |
| 712                          | 0.04035        | 0.04006 | 0.03978 | 0.03951 | 0.03924 | 0.03897 |
| 714                          | 4046           | 4018    | 3989    | 3962    | 3935    | 3908    |
| 716                          | 4057           | 4029    | 4001    | 3973    | 3946    | 3919    |
| 718                          | 4068           | 4040    | 4012    | 3984    | 3957    | 3930    |
| 720                          | 4080           | 4051    | 4023    | 3995    | 3968    | 3941    |



**TABLE 2.18** Molar Equivalent of One Liter of Gas at Various Temperatures and Pressures (*Continued*)

| Pressure<br>mm of<br>mercury | Temperature °C |         |         |         |         |         |
|------------------------------|----------------|---------|---------|---------|---------|---------|
|                              | 10°            | 12°     | 14°     | 16°     | 18°     | 20°     |
| 722                          | 0.04091        | 0.04063 | 0.04034 | 0.04006 | 0.03979 | 0.03952 |
| 724                          | 4103           | 4074    | 4045    | 4017    | 3990    | 3963    |
| 726                          | 4114           | 4085    | 4057    | 4028    | 4001    | 3973    |
| 728                          | 4125           | 4096    | 4068    | 4040    | 4012    | 3984    |
| 730                          | 4136           | 4108    | 4079    | 4051    | 4023    | 3995    |
| 732                          | 0.04148        | 0.04119 | 0.04090 | 0.04062 | 0.04034 | 0.04006 |
| 734                          | 4159           | 4130    | 4101    | 4073    | 4045    | 4017    |
| 736                          | 4171           | 4141    | 4112    | 4084    | 4056    | 4028    |
| 738                          | 4182           | 4153    | 4124    | 4095    | 4067    | 4039    |
| 740                          | 4193           | 4164    | 4135    | 4106    | 4078    | 4050    |
| 742                          | 0.04204        | 0.04175 | 0.04146 | 0.04117 | 0.04089 | 0.04061 |
| 744                          | 4216           | 4186    | 4157    | 4128    | 4100    | 4072    |
| 746                          | 4227           | 4198    | 4168    | 4139    | 4111    | 4038    |
| 748                          | 4239           | 4209    | 4179    | 4151    | 4122    | 4094    |
| 750                          | 4250           | 4220    | 4191    | 4162    | 4133    | 4105    |
| 752                          | 0.04261        | 0.04231 | 0.04202 | 0.04173 | 0.04144 | 0.04116 |
| 754                          | 4273           | 4243    | 4213    | 4184    | 4155    | 4127    |
| 756                          | 4284           | 4254    | 4224    | 4195    | 4166    | 4138    |
| 758                          | 4295           | 4265    | 4235    | 4206    | 4177    | 4149    |
| 760                          | 4307           | 4276    | 4247    | 4217    | 4188    | 4160    |
| 762                          | 0.04318        | 0.04287 | 0.04258 | 0.04228 | 0.04199 | 0.04171 |
| 764                          | 4329           | 4299    | 4269    | 4239    | 4210    | 4181    |
| 766                          | 4341           | 4310    | 4280    | 4250    | 4221    | 4192    |
| 768                          | 4352           | 4321    | 4291    | 4262    | 4232    | 4203    |
| 770                          | 4363           | 4333    | 4302    | 4273    | 4243    | 4214    |
| 772                          | 0.04375        | 0.04344 | 0.04314 | 0.04284 | 0.04254 | 0.04225 |
| 774                          | 4386           | 4355    | 4325    | 4295    | 4265    | 4236    |
| 776                          | 4397           | 4366    | 4336    | 4306    | 4276    | 4247    |
| 778                          | 4409           | 4378    | 4347    | 4317    | 4287    | 4258    |
| 780                          | 4420           | 4389    | 4358    | 4328    | 4298    | 4269    |
| Pressure<br>mm of<br>mercury | Temperature °C |         |         |         |         |         |
|                              | 22°            | 24°     | 26°     | 28°     | 30°     | 32°     |
| 655                          | 0.03561        | 0.03537 | 0.03515 | 0.03490 | 0.03467 | 0.03444 |
| 660                          | 3588           | 3564    | 3541    | 3516    | 3493    | 3470    |
| 665                          | 3614           | 3591    | 3568    | 3543    | 3520    | 3496    |
| 670                          | 3642           | 3618    | 3595    | 3569    | 3546    | 3523    |
| 675                          | 3669           | 3645    | 3622    | 3596    | 3572    | 3549    |
| 680                          | 0.03697        | 0.03672 | 0.03649 | 0.03623 | 0.03599 | 0.03575 |
| 685                          | 3724           | 3699    | 3676    | 3649    | 3625    | 3602    |
| 690                          | 3751           | 3726    | 3702    | 3676    | 3652    | 3628    |
| 695                          | 3778           | 3753    | 3729    | 3703    | 3678    | 3654    |
| 700                          | 3805           | 3780    | 3756    | 3729    | 3705    | 3680    |

**TABLE 2.18** Molar Equivalent of One Liter of Gas at Various Temperatures and Pressures (*Continued*)

| Pressure<br>mm of<br>mercury | Temperature °C |         |         |         |         |         |
|------------------------------|----------------|---------|---------|---------|---------|---------|
|                              | 22°            | 24°     | 26°     | 28°     | 30°     | 32°     |
| 702                          | 0.03816        | 0.03790 | 0.03767 | 0.03740 | 0.03715 | 0.03691 |
| 704                          | 3827           | 3801    | 3777    | 3750    | 3726    | 3701    |
| 706                          | 3838           | 3812    | 3788    | 3761    | 3736    | 3712    |
| 708                          | 3849           | 3823    | 3799    | 3772    | 3747    | 3722    |
| 710                          | 3860           | 3834    | 3810    | 3783    | 3758    | 3733    |
| 712                          | 0.03870        | 0.03844 | 0.03820 | 0.03793 | 0.03768 | 0.03744 |
| 714                          | 3881           | 3855    | 3831    | 3804    | 3779    | 3754    |
| 716                          | 3892           | 3866    | 3842    | 3815    | 3789    | 3765    |
| 718                          | 3902           | 3877    | 3853    | 3825    | 3800    | 3775    |
| 720                          | 3914           | 3888    | 3863    | 3836    | 3811    | 3786    |
| 722                          | 0.03925        | 0.03898 | 0.03874 | 0.03847 | 0.03821 | 0.03796 |
| 724                          | 3936           | 3909    | 3885    | 3857    | 3832    | 3807    |
| 726                          | 3947           | 3920    | 3896    | 3868    | 3842    | 3817    |
| 728                          | 3957           | 3931    | 3906    | 3878    | 3853    | 3828    |
| 730                          | 3968           | 3941    | 3917    | 3889    | 3863    | 3838    |
| 732                          | 0.03979        | 0.03952 | 0.03928 | 0.03900 | 0.03874 | 0.03849 |
| 734                          | 3990           | 3963    | 3938    | 3910    | 3885    | 3859    |
| 736                          | 4001           | 3974    | 3949    | 3921    | 3895    | 3870    |
| 738                          | 4012           | 3985    | 3960    | 3932    | 3906    | 3880    |
| 740                          | 4023           | 3995    | 3971    | 3942    | 3916    | 3891    |
| 742                          | 0.04033        | 0.04006 | 0.03981 | 0.03953 | 0.03927 | 0.03901 |
| 744                          | 4044           | 4017    | 3992    | 3964    | 3938    | 3912    |
| 746                          | 4055           | 4028    | 4003    | 3974    | 3948    | 3922    |
| 748                          | 4066           | 4039    | 4014    | 3985    | 3959    | 3933    |
| 750                          | 4077           | 4049    | 4024    | 3996    | 3969    | 3943    |
| 752                          | 0.04088        | 0.04060 | 0.04035 | 0.04006 | 0.03980 | 0.03954 |
| 754                          | 4099           | 4071    | 4046    | 4017    | 3991    | 3964    |
| 756                          | 4110           | 4082    | 4056    | 4028    | 4001    | 3975    |
| 758                          | 4121           | 4093    | 4067    | 4038    | 4012    | 3985    |
| 760                          | 4131           | 4103    | 4078    | 4049    | 4022    | 3996    |
| 762                          | 0.04142        | 4114    | 4089    | 4060    | 4033    | 4006    |
| 764                          | 4153           | 4125    | 4099    | 4070    | 4043    | 4017    |
| 766                          | 4164           | 4136    | 4110    | 4081    | 4054    | 4027    |
| 768                          | 4175           | 4147    | 4121    | 4092    | 4065    | 4038    |
| 770                          | 4186           | 4158    | 4132    | 4102    | 4075    | 4048    |
| 772                          | 0.04197        | 0.04168 | 0.04142 | 0.04113 | 0.04086 | 0.04059 |
| 774                          | 4207           | 4179    | 4153    | 4124    | 4096    | 4070    |
| 776                          | 4218           | 4190    | 4164    | 4134    | 4107    | 4080    |
| 778                          | 4229           | 4201    | 4175    | 4145    | 4117    | 4091    |
| 780                          | 4240           | 4211    | 4185    | 4155    | 4128    | 4101    |

**TABLE 2.19** Factors for Reducing Gas Volumes to Normal (Standard) Temperature and Pressure (760 mmHg)

*Examples:* (a) 20 mL of dry gas at 22°C and 730 mm =  $20 \times 0.8888 = 17.78$  mL at 0°C and 760 mm. (b) 20 mL of a gas over water at 22° and 730 mm =  $20 \times$  (factor corrected for aqueous tension; i.e., 730 – 19.8 or 710.2 mm) = 20 mL of dry gas at 22° and 710.2 mm =  $20 \times 0.86475 = 17.30$  mL at 0°C and 760 mm. Mass in milligrams of 1 mL of gas at S.T.P.: acetylene, 1.173; carbon dioxide, 1.9769; hydrogen, 0.0899; nitric oxide (NO), 1.3402; nitrogen, 1.25057; oxygen, 1.42904.

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |        |        |        |        |        |
|------------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|
|                              | 10°            | 11°    | 12°    | 13°    | 14°    | 15°    | 16°    | 17°    |
| 670                          | 0.8504         | 0.8474 | 0.8445 | 0.8415 | 0.8386 | 0.8357 | 0.8328 | 0.8299 |
| 672                          | 0.8530         | 0.8500 | 0.8470 | 0.8440 | 0.8411 | 0.8382 | 0.8353 | 0.8324 |
| 674                          | 0.8555         | 0.8525 | 0.8495 | 0.8465 | 0.8436 | 0.8407 | 0.8377 | 0.8349 |
| 676                          | 0.8580         | 0.8550 | 0.8520 | 0.8490 | 0.8461 | 0.8431 | 0.8402 | 0.8373 |
| 678                          | 0.8606         | 0.8576 | 0.8545 | 0.8516 | 0.8486 | 0.8456 | 0.8427 | 0.8398 |
| 680                          | 0.8631         | 0.8601 | 0.8571 | 0.8541 | 0.8511 | 0.8481 | 0.8452 | 0.8423 |
| 682                          | 0.8657         | 0.8626 | 0.8596 | 0.8566 | 0.8536 | 0.8506 | 0.8477 | 0.8448 |
| 684                          | 0.8682         | 0.8651 | 0.8621 | 0.8591 | 0.8561 | 0.8531 | 0.8502 | 0.8472 |
| 686                          | 0.8707         | 0.8677 | 0.8646 | 0.8616 | 0.8586 | 0.8556 | 0.8527 | 0.8497 |
| 688                          | 0.8733         | 0.8702 | 0.8672 | 0.8641 | 0.8611 | 0.8581 | 0.8551 | 0.8522 |
| 690                          | 0.8758         | 0.8727 | 0.8697 | 0.8666 | 0.8636 | 0.8606 | 0.8576 | 0.8547 |
| 692                          | 0.8784         | 0.8753 | 0.8722 | 0.8691 | 0.8661 | 0.8631 | 0.8601 | 0.8572 |
| 694                          | 0.8809         | 0.8778 | 0.8747 | 0.8717 | 0.8686 | 0.8656 | 0.8626 | 0.8596 |
| 696                          | 0.8834         | 0.8803 | 0.8772 | 0.8742 | 0.8711 | 0.8681 | 0.8651 | 0.8621 |
| 698                          | 0.8860         | 0.8828 | 0.8798 | 0.8767 | 0.8736 | 0.8706 | 0.8676 | 0.8646 |
| 700                          | 0.8885         | 0.8854 | 0.8823 | 0.8792 | 0.8761 | 0.8731 | 0.8700 | 0.8671 |
| 702                          | 0.8910         | 0.8879 | 0.8848 | 0.8817 | 0.8786 | 0.8756 | 0.8725 | 0.8695 |
| 704                          | 0.8936         | 0.8904 | 0.8873 | 0.8842 | 0.8811 | 0.8781 | 0.8750 | 0.8720 |
| 706                          | 0.8961         | 0.8930 | 0.8898 | 0.8867 | 0.8836 | 0.8806 | 0.8775 | 0.8745 |
| 708                          | 0.8987         | 0.8955 | 0.8924 | 0.8892 | 0.8861 | 0.8831 | 0.8800 | 0.8770 |
| 710                          | 0.9012         | 0.8980 | 0.8949 | 0.8917 | 0.8886 | 0.8856 | 0.8825 | 0.8794 |
| 712                          | 0.9037         | 0.9006 | 0.8974 | 0.8943 | 0.8911 | 0.8880 | 0.8850 | 0.8819 |
| 714                          | 0.9063         | 0.9031 | 0.8999 | 0.8968 | 0.8936 | 0.8905 | 0.8875 | 0.8844 |
| 716                          | 0.9088         | 0.9056 | 0.9024 | 0.8993 | 0.8961 | 0.8930 | 0.8899 | 0.8869 |
| 718                          | 0.9114         | 0.9081 | 0.9050 | 0.9018 | 0.8987 | 0.8955 | 0.8924 | 0.8894 |
| 720                          | 0.9139         | 0.9107 | 0.9075 | 0.9043 | 0.9012 | 0.8980 | 0.8949 | 0.8918 |
| 722                          | 0.9164         | 0.9132 | 0.9100 | 0.9068 | 0.9037 | 0.9005 | 0.8974 | 0.8943 |
| 724                          | 0.9190         | 0.9157 | 0.9125 | 0.9093 | 0.9062 | 0.9030 | 0.8999 | 0.8968 |
| 726                          | 0.9215         | 0.9183 | 0.9151 | 0.9118 | 0.9087 | 0.9055 | 0.9024 | 0.8993 |
| 728                          | 0.9241         | 0.9208 | 0.9176 | 0.9144 | 0.9112 | 0.9080 | 0.9049 | 0.9017 |
| 730                          | 0.9266         | 0.9233 | 0.9201 | 0.9169 | 0.9137 | 0.9105 | 0.9073 | 0.9042 |
| 732                          | 0.9291         | 0.9259 | 0.9226 | 0.9194 | 0.9162 | 0.9130 | 0.9098 | 0.9067 |
| 734                          | 0.9317         | 0.9284 | 0.9251 | 0.9219 | 0.9187 | 0.9155 | 0.9123 | 0.9092 |
| 736                          | 0.9342         | 0.9309 | 0.9277 | 0.9244 | 0.9212 | 0.9180 | 0.9148 | 0.9117 |
| 738                          | 0.9368         | 0.9334 | 0.9302 | 0.9269 | 0.9237 | 0.9205 | 0.9173 | 0.9141 |
| 740                          | 0.9393         | 0.9360 | 0.9327 | 0.9294 | 0.9262 | 0.9230 | 0.9198 | 0.9166 |
| 742                          | 0.9418         | 0.9385 | 0.9352 | 0.9319 | 0.9287 | 0.9255 | 0.9223 | 0.9191 |
| 744                          | 0.9444         | 0.9410 | 0.9377 | 0.9345 | 0.9312 | 0.9280 | 0.9248 | 0.9216 |
| 746                          | 0.9469         | 0.9436 | 0.9403 | 0.9370 | 0.9337 | 0.9305 | 0.9272 | 0.9240 |
| 748                          | 0.9494         | 0.9461 | 0.9428 | 0.9395 | 0.9362 | 0.9329 | 0.9297 | 0.9265 |

**TABLE 2.19** Factors for Reducing Gas Volumes to Normal (Standard) Temperature and Pressure *(Continued)*

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |        |        |        |        |        |
|------------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|
|                              | 10°            | 11°    | 12°    | 13°    | 14°    | 15°    | 16°    | 17°    |
| 750                          | 0.9520         | 0.9486 | 0.9453 | 0.9420 | 0.9387 | 0.9354 | 0.9322 | 0.9290 |
| 752                          | 0.9545         | 0.9511 | 0.9478 | 0.9445 | 0.9412 | 0.9379 | 0.9347 | 0.9315 |
| 754                          | 0.9571         | 0.9537 | 0.9504 | 0.9470 | 0.9437 | 0.9404 | 0.9372 | 0.9339 |
| 756                          | 0.9596         | 0.9562 | 0.9529 | 0.9495 | 0.9462 | 0.9429 | 0.9397 | 0.9364 |
| 758                          | 0.9621         | 0.9587 | 0.9554 | 0.9520 | 0.9487 | 0.9454 | 0.9422 | 0.9389 |
| 760                          | 0.9647         | 0.9613 | 0.9579 | 0.9546 | 0.9512 | 0.9479 | 0.9446 | 0.9414 |
| 762                          | 0.9672         | 0.9638 | 0.9604 | 0.9571 | 0.9537 | 0.9504 | 0.9471 | 0.9439 |
| 764                          | 0.9698         | 0.9663 | 0.9630 | 0.9596 | 0.9562 | 0.9529 | 0.9496 | 0.9463 |
| 766                          | 0.9723         | 0.9689 | 0.9655 | 0.9620 | 0.9587 | 0.9554 | 0.9521 | 0.9488 |
| 768                          | 0.9748         | 0.9714 | 0.9680 | 0.9646 | 0.9612 | 0.9579 | 0.9546 | 0.9513 |
| 770                          | 0.9774         | 0.9739 | 0.9705 | 0.9671 | 0.9637 | 0.9604 | 0.9571 | 0.9538 |
| 772                          | 0.9799         | 0.9764 | 0.9730 | 0.9696 | 0.9662 | 0.9629 | 0.9596 | 0.9562 |
| 774                          | 0.9825         | 0.9790 | 0.9756 | 0.9721 | 0.9687 | 0.9654 | 0.9620 | 0.9587 |
| 776                          | 0.9850         | 0.9815 | 0.9781 | 0.9746 | 0.9712 | 0.9679 | 0.9645 | 0.9612 |
| 778                          | 0.9875         | 0.9840 | 0.9806 | 0.9772 | 0.9737 | 0.9704 | 0.9670 | 0.9637 |
| 780                          | 0.9901         | 0.9866 | 0.9831 | 0.9797 | 0.9763 | 0.9729 | 0.9695 | 0.9662 |
| 782                          | 0.9926         | 0.9891 | 0.9856 | 0.9822 | 0.9788 | 0.9754 | 0.9720 | 0.9686 |
| 784                          | 0.9952         | 0.9916 | 0.9882 | 0.9847 | 0.9813 | 0.9778 | 0.9745 | 0.9711 |
| 786                          | 0.9977         | 0.9942 | 0.9907 | 0.9872 | 0.9838 | 0.9803 | 0.9770 | 0.9736 |
| 788                          | 1.0002         | 0.9967 | 0.9932 | 0.9897 | 0.9863 | 0.9828 | 0.9794 | 0.9761 |
| Pressure<br>mm of<br>mercury | Temperature °C |        |        |        |        |        |        |        |
|                              | 18°            | 19°    | 20°    | 21°    | 22°    | 23°    | 24°    | 25°    |
| 670                          | 0.8270         | 0.8242 | 0.8214 | 0.8186 | 0.8158 | 0.8131 | 0.8103 | 0.8076 |
| 672                          | 0.8295         | 0.8267 | 0.8239 | 0.8211 | 0.8183 | 0.8155 | 0.8128 | 0.8100 |
| 674                          | 0.8320         | 0.8291 | 0.8263 | 0.8235 | 0.8207 | 0.8179 | 0.8152 | 0.8124 |
| 676                          | 0.8345         | 0.8316 | 0.8288 | 0.8259 | 0.8231 | 0.8204 | 0.8176 | 0.8149 |
| 678                          | 0.8369         | 0.8341 | 0.8312 | 0.8284 | 0.8256 | 0.8228 | 0.8200 | 0.8173 |
| 680                          | 0.8394         | 0.8365 | 0.8337 | 0.8308 | 0.8280 | 0.8252 | 0.8224 | 0.8197 |
| 682                          | 0.8419         | 0.8390 | 0.8361 | 0.8333 | 0.8304 | 0.8276 | 0.8249 | 0.8221 |
| 684                          | 0.8443         | 0.8414 | 0.8386 | 0.8357 | 0.8329 | 0.8301 | 0.8273 | 0.8245 |
| 686                          | 0.8468         | 0.8439 | 0.8410 | 0.8382 | 0.8353 | 0.8325 | 0.8297 | 0.8269 |
| 688                          | 0.8493         | 0.8464 | 0.8435 | 0.8406 | 0.8378 | 0.8349 | 0.8321 | 0.8293 |
| 690                          | 0.8517         | 0.8488 | 0.8459 | 0.8430 | 0.8402 | 0.8373 | 0.8345 | 0.8317 |
| 692                          | 0.8542         | 0.8513 | 0.8484 | 0.8455 | 0.8426 | 0.8398 | 0.8369 | 0.8341 |
| 694                          | 0.8567         | 0.8537 | 0.8508 | 0.8479 | 0.8451 | 0.8422 | 0.8394 | 0.8366 |
| 696                          | 0.8591         | 0.8562 | 0.8533 | 0.8504 | 0.8475 | 0.8446 | 0.8418 | 0.8390 |
| 698                          | 0.8616         | 0.8587 | 0.8557 | 0.8528 | 0.8499 | 0.8471 | 0.8442 | 0.8414 |
| 700                          | 0.8641         | 0.8611 | 0.8582 | 0.8553 | 0.8524 | 0.8495 | 0.8466 | 0.8438 |
| 702                          | 0.8665         | 0.8636 | 0.8606 | 0.8577 | 0.8547 | 0.8519 | 0.8490 | 0.8462 |
| 704                          | 0.8690         | 0.8660 | 0.8631 | 0.8602 | 0.8572 | 0.8543 | 0.8515 | 0.8486 |
| 706                          | 0.8715         | 0.8685 | 0.8655 | 0.8626 | 0.8597 | 0.8568 | 0.8539 | 0.8510 |
| 708                          | 0.8740         | 0.8710 | 0.8680 | 0.8650 | 0.8621 | 0.8592 | 0.8563 | 0.8534 |

**TABLE 2.19** Factors for Reducing Gas Volumes to Normal (Standard) Temperature and Pressure (*Continued*)

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |        |        |        |        |        |
|------------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|
|                              | 18°            | 19°    | 20°    | 21°    | 22°    | 23°    | 24°    | 25°    |
| 710                          | 0.8764         | 0.8734 | 0.8704 | 0.8675 | 0.8645 | 0.8616 | 0.8587 | 0.8558 |
| 712                          | 0.8789         | 0.8759 | 0.8729 | 0.8699 | 0.8670 | 0.8640 | 0.8611 | 0.8582 |
| 714                          | 0.8814         | 0.8783 | 0.8753 | 0.8724 | 0.8694 | 0.8665 | 0.8636 | 0.8607 |
| 716                          | 0.8838         | 0.8808 | 0.8778 | 0.8748 | 0.8718 | 0.8689 | 0.8660 | 0.8631 |
| 718                          | 0.8863         | 0.8833 | 0.8802 | 0.8773 | 0.8743 | 0.8713 | 0.8684 | 0.8655 |
| 720                          | 0.8888         | 0.8857 | 0.8827 | 0.8797 | 0.8767 | 0.8738 | 0.8708 | 0.8679 |
| 722                          | 0.8912         | 0.8882 | 0.8852 | 0.8821 | 0.8792 | 0.8762 | 0.8732 | 0.8703 |
| 724                          | 0.8937         | 0.8906 | 0.8876 | 0.8846 | 0.8816 | 0.8786 | 0.8757 | 0.8727 |
| 726                          | 0.8962         | 0.8931 | 0.8901 | 0.8870 | 0.8840 | 0.8810 | 0.8781 | 0.8751 |
| 728                          | 0.8986         | 0.8956 | 0.8925 | 0.8895 | 0.8865 | 0.8835 | 0.8805 | 0.8775 |
| 730                          | 0.9011         | 0.8980 | 0.8950 | 0.8919 | 0.8889 | 0.8859 | 0.8829 | 0.8799 |
| 732                          | 0.9036         | 0.9005 | 0.8974 | 0.8944 | 0.8913 | 0.8883 | 0.8853 | 0.8824 |
| 734                          | 0.9060         | 0.9029 | 0.8999 | 0.8968 | 0.8938 | 0.8907 | 0.8877 | 0.8848 |
| 736                          | 0.9085         | 0.9054 | 0.9023 | 0.8992 | 0.8962 | 0.8932 | 0.8902 | 0.8872 |
| 738                          | 0.9110         | 0.9079 | 0.9048 | 0.9017 | 0.8986 | 0.8956 | 0.8926 | 0.8896 |
| 740                          | 0.9135         | 0.9103 | 0.9072 | 0.9041 | 0.9011 | 0.8980 | 0.8950 | 0.8920 |
| 742                          | 0.9159         | 0.9128 | 0.9097 | 0.9066 | 0.9035 | 0.9005 | 0.8974 | 0.8944 |
| 744                          | 0.9184         | 0.9153 | 0.9121 | 0.9090 | 0.9059 | 0.9029 | 0.8998 | 0.8968 |
| 746                          | 0.9209         | 0.9177 | 0.9146 | 0.9115 | 0.9084 | 0.9053 | 0.9023 | 0.8992 |
| 748                          | 0.9233         | 0.9202 | 0.9170 | 0.9139 | 0.9108 | 0.9077 | 0.9047 | 0.9016 |
| 750                          | 0.9258         | 0.9226 | 0.9195 | 0.9164 | 0.9132 | 0.9102 | 0.9071 | 0.9041 |
| 752                          | 0.9283         | 0.9251 | 0.9219 | 0.9188 | 0.9157 | 0.9126 | 0.9095 | 0.9065 |
| 754                          | 0.9307         | 0.9276 | 0.9244 | 0.9212 | 0.9181 | 0.9150 | 0.9119 | 0.9089 |
| 756                          | 0.9332         | 0.9300 | 0.9268 | 0.9237 | 0.9206 | 0.9174 | 0.9144 | 0.9113 |
| 758                          | 0.9357         | 0.9325 | 0.9293 | 0.9261 | 0.9230 | 0.9199 | 0.9168 | 0.9137 |
| 760                          | 0.9381         | 0.9349 | 0.9317 | 0.9286 | 0.9254 | 0.9223 | 0.9192 | 0.9161 |
| 762                          | 0.9406         | 0.9374 | 0.9342 | 0.9310 | 0.9279 | 0.9247 | 0.9216 | 0.9185 |
| 764                          | 0.9431         | 0.9399 | 0.9366 | 0.9335 | 0.9303 | 0.9272 | 0.9240 | 0.9209 |
| 766                          | 0.9456         | 0.9423 | 0.9391 | 0.9359 | 0.9327 | 0.9296 | 0.9265 | 0.9233 |
| 768                          | 0.9480         | 0.9448 | 0.9415 | 0.9383 | 0.9352 | 0.9320 | 0.9289 | 0.9258 |
| 770                          | 0.9505         | 0.9472 | 0.9440 | 0.9408 | 0.9376 | 0.9344 | 0.9313 | 0.9282 |
| 772                          | 0.9530         | 0.9497 | 0.9464 | 0.9432 | 0.9400 | 0.9369 | 0.9337 | 0.9306 |
| 774                          | 0.9554         | 0.9522 | 0.9489 | 0.9457 | 0.9425 | 0.9393 | 0.9361 | 0.9330 |
| 776                          | 0.9579         | 0.9546 | 0.9514 | 0.9481 | 0.9449 | 0.9417 | 0.9385 | 0.9354 |
| 778                          | 0.9604         | 0.9571 | 0.9538 | 0.9506 | 0.9473 | 0.9441 | 0.9410 | 0.9378 |
| 780                          | 0.9628         | 0.9595 | 0.9563 | 0.9530 | 0.9498 | 0.9466 | 0.9434 | 0.9402 |
| 782                          | 0.9653         | 0.9620 | 0.9587 | 0.9555 | 0.9522 | 0.9490 | 0.9458 | 0.9426 |
| 784                          | 0.9678         | 0.9645 | 0.9612 | 0.9579 | 0.9546 | 0.9514 | 0.9482 | 0.9450 |
| 786                          | 0.9702         | 0.9669 | 0.9636 | 0.9603 | 0.9571 | 0.9538 | 0.9506 | 0.9474 |
| 788                          | 0.9727         | 0.9694 | 0.9661 | 0.9628 | 0.9595 | 0.9563 | 0.9531 | 0.9499 |

**TABLE 2.19** Factors for Reducing Gas Volumes to Normal (Standard) Temperature and Pressure *(Continued)*

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |        |        |        |        |        |
|------------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|
|                              | 26°            | 27°    | 28°    | 29°    | 30°    | 31°    | 32°    | 33°    |
| 670                          | 0.8049         | 0.8022 | 0.7996 | 0.7969 | 0.7943 | 0.7917 | 0.7891 | 0.7865 |
| 672                          | 0.8073         | 0.8046 | 0.8020 | 0.7993 | 0.7967 | 0.7940 | 0.7914 | 0.7889 |
| 674                          | 0.8097         | 0.8070 | 0.8043 | 0.8017 | 0.7990 | 0.7964 | 0.7938 | 0.7912 |
| 676                          | 0.8121         | 0.8094 | 0.8067 | 0.8041 | 0.8014 | 0.7988 | 0.7962 | 0.7936 |
| 678                          | 0.8145         | 0.8118 | 0.8091 | 0.8064 | 0.8038 | 0.8011 | 0.7985 | 0.7959 |
| 680                          | 0.8169         | 0.8142 | 0.8115 | 0.8088 | 0.8061 | 0.8035 | 0.8009 | 0.7982 |
| 682                          | 0.8193         | 0.8166 | 0.8139 | 0.8112 | 0.8085 | 0.8059 | 0.8032 | 0.8006 |
| 684                          | 0.8217         | 0.8190 | 0.8163 | 0.8136 | 0.8109 | 0.8082 | 0.8056 | 0.8029 |
| 686                          | 0.8241         | 0.8214 | 0.8187 | 0.8160 | 0.8133 | 0.8106 | 0.8079 | 0.8053 |
| 688                          | 0.8265         | 0.8238 | 0.8211 | 0.8183 | 0.8156 | 0.8129 | 0.8103 | 0.8076 |
| 690                          | 0.8289         | 0.8262 | 0.8234 | 0.8207 | 0.8180 | 0.8153 | 0.8126 | 0.8100 |
| 692                          | 0.8313         | 0.8286 | 0.8258 | 0.8231 | 0.8204 | 0.8177 | 0.8150 | 0.8123 |
| 694                          | 0.8338         | 0.8310 | 0.8282 | 0.8255 | 0.8227 | 0.8200 | 0.8174 | 0.8147 |
| 696                          | 0.8362         | 0.8334 | 0.8306 | 0.8278 | 0.8251 | 0.8224 | 0.8197 | 0.8170 |
| 698                          | 0.8386         | 0.8358 | 0.8330 | 0.8302 | 0.8275 | 0.8248 | 0.8221 | 0.8194 |
| 700                          | 0.8410         | 0.8382 | 0.8354 | 0.8326 | 0.8299 | 0.8271 | 0.8244 | 0.8217 |
| 702                          | 0.8434         | 0.8406 | 0.8378 | 0.8350 | 0.8322 | 0.8295 | 0.8268 | 0.8241 |
| 704                          | 0.8458         | 0.8429 | 0.8401 | 0.8374 | 0.8346 | 0.8319 | 0.8291 | 0.8264 |
| 706                          | 0.8482         | 0.8453 | 0.8425 | 0.8397 | 0.8370 | 0.8342 | 0.8315 | 0.8288 |
| 708                          | 0.8506         | 0.8477 | 0.8449 | 0.8421 | 0.8393 | 0.8366 | 0.8338 | 0.8311 |
| 710                          | 0.8530         | 0.8501 | 0.8473 | 0.8445 | 0.8417 | 0.8389 | 0.8362 | 0.8335 |
| 712                          | 0.8554         | 0.8525 | 0.8497 | 0.8469 | 0.8441 | 0.8413 | 0.8386 | 0.8358 |
| 714                          | 0.8578         | 0.8549 | 0.8521 | 0.8493 | 0.8465 | 0.8437 | 0.8409 | 0.8382 |
| 716                          | 0.8602         | 0.8573 | 0.8545 | 0.8516 | 0.8488 | 0.8460 | 0.8433 | 0.8405 |
| 718                          | 0.8626         | 0.8597 | 0.8569 | 0.8540 | 0.8512 | 0.8484 | 0.8456 | 0.8429 |
| 720                          | 0.8650         | 0.8621 | 0.8592 | 0.8564 | 0.8536 | 0.8508 | 0.8480 | 0.8452 |
| 722                          | 0.8674         | 0.8645 | 0.8616 | 0.8588 | 0.8559 | 0.8531 | 0.8503 | 0.8475 |
| 724                          | 0.8698         | 0.8669 | 0.8640 | 0.8612 | 0.8583 | 0.8555 | 0.8527 | 0.8499 |
| 726                          | 0.8722         | 0.8693 | 0.8664 | 0.8635 | 0.8607 | 0.8579 | 0.8550 | 0.8522 |
| 728                          | 0.8746         | 0.8717 | 0.8688 | 0.8659 | 0.8631 | 0.8602 | 0.8574 | 0.8546 |
| 730                          | 0.8770         | 0.8741 | 0.8712 | 0.8683 | 0.8654 | 0.8626 | 0.8598 | 0.8569 |
| 732                          | 0.8794         | 0.8765 | 0.8736 | 0.8707 | 0.8678 | 0.8649 | 0.8621 | 0.8593 |
| 734                          | 0.8818         | 0.8789 | 0.8759 | 0.8730 | 0.8702 | 0.8673 | 0.8645 | 0.8616 |
| 736                          | 0.8842         | 0.8813 | 0.8783 | 0.8754 | 0.8725 | 0.8697 | 0.8668 | 0.8640 |
| 738                          | 0.8866         | 0.8837 | 0.8807 | 0.8778 | 0.8749 | 0.8720 | 0.8692 | 0.8663 |
| 740                          | 0.8890         | 0.8861 | 0.8831 | 0.8802 | 0.8773 | 0.8744 | 0.8715 | 0.8687 |
| 742                          | 0.8914         | 0.8884 | 0.8855 | 0.8826 | 0.8796 | 0.8768 | 0.8739 | 0.8710 |
| 744                          | 0.8938         | 0.8908 | 0.8879 | 0.8849 | 0.8820 | 0.8791 | 0.8762 | 0.8734 |
| 746                          | 0.8962         | 0.8932 | 0.8903 | 0.8873 | 0.8844 | 0.8815 | 0.8786 | 0.8757 |
| 748                          | 0.8986         | 0.8956 | 0.8927 | 0.8897 | 0.8868 | 0.8838 | 0.8809 | 0.8781 |
| 750                          | 0.9010         | 0.8980 | 0.8950 | 0.8921 | 0.8891 | 0.8862 | 0.8833 | 0.8804 |
| 752                          | 0.9034         | 0.9004 | 0.8974 | 0.8945 | 0.8915 | 0.8886 | 0.8857 | 0.8828 |
| 754                          | 0.9058         | 0.9028 | 0.8998 | 0.8968 | 0.8939 | 0.8909 | 0.8880 | 0.8851 |
| 756                          | 0.9082         | 0.9052 | 0.9022 | 0.8992 | 0.8962 | 0.8933 | 0.8904 | 0.8875 |
| 758                          | 0.9106         | 0.9076 | 0.9046 | 0.9016 | 0.8986 | 0.8957 | 0.8927 | 0.8898 |

**TABLE 2.19** Factors for Reducing Gas Volumes to Normal (Standard) Temperature and Pressure *(Continued)*

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |        |        |        |        |        |
|------------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|
|                              | 26°            | 27°    | 28°    | 29°    | 30°    | 31°    | 32°    | 33°    |
| 760                          | 0.9130         | 0.9100 | 0.9070 | 0.9040 | 0.9010 | 0.8980 | 0.8951 | 0.8922 |
| 762                          | 0.9154         | 0.9124 | 0.9094 | 0.9064 | 0.9034 | 0.9004 | 0.8974 | 0.8945 |
| 764                          | 0.9178         | 0.9148 | 0.9118 | 0.9087 | 0.9057 | 0.9028 | 0.8998 | 0.8969 |
| 766                          | 0.9202         | 0.9172 | 0.9141 | 0.9111 | 0.9081 | 0.9051 | 0.9021 | 0.8992 |
| 768                          | 0.9227         | 0.9196 | 0.9165 | 0.9135 | 0.9105 | 0.9075 | 0.9045 | 0.9015 |
| 770                          | 0.9251         | 0.9220 | 0.9189 | 0.9159 | 0.9128 | 0.9098 | 0.9069 | 0.9039 |
| 772                          | 0.9275         | 0.9244 | 0.9213 | 0.9182 | 0.9152 | 0.9122 | 0.9092 | 0.9062 |
| 774                          | 0.9299         | 0.9268 | 0.9237 | 0.9206 | 0.9176 | 0.9146 | 0.9116 | 0.9086 |
| 776                          | 0.9323         | 0.9292 | 0.9261 | 0.9230 | 0.9200 | 0.9169 | 0.9139 | 0.9109 |
| 778                          | 0.9347         | 0.9316 | 0.9285 | 0.9254 | 0.9223 | 0.9193 | 0.9163 | 0.9133 |
| 780                          | 0.9371         | 0.9340 | 0.9308 | 0.9278 | 0.9247 | 0.9217 | 0.9186 | 0.9156 |
| 782                          | 0.9395         | 0.9363 | 0.9332 | 0.9301 | 0.9271 | 0.9240 | 0.9210 | 0.9180 |
| 784                          | 0.9419         | 0.9387 | 0.9356 | 0.9325 | 0.9294 | 0.9264 | 0.9233 | 0.9203 |
| 786                          | 0.9443         | 0.9411 | 0.9380 | 0.9349 | 0.9318 | 0.9287 | 0.9257 | 0.9227 |
| 788                          | 0.9467         | 0.9435 | 0.9404 | 0.9373 | 0.9342 | 0.9311 | 0.9281 | 0.9250 |

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |
|------------------------------|----------------|--------|--------|
|                              | 34°            | 35°    | 36°    |
| 670                          | 0.7839         | 0.7814 | 0.7789 |
| 672                          | 0.7863         | 0.7837 | 0.7812 |
| 674                          | 0.7886         | 0.7861 | 0.7835 |
| 676                          | 0.7910         | 0.7884 | 0.7858 |
| 678                          | 0.7933         | 0.7907 | 0.7882 |
| 680                          | 0.7956         | 0.7931 | 0.7905 |
| 682                          | 0.7980         | 0.7954 | 0.7928 |
| 684                          | 0.8003         | 0.7977 | 0.7951 |
| 686                          | 0.8027         | 0.8001 | 0.7975 |
| 688                          | 0.8050         | 0.8024 | 0.7998 |
| 690                          | 0.8073         | 0.8047 | 0.8021 |
| 692                          | 0.8097         | 0.8071 | 0.8044 |
| 694                          | 0.8120         | 0.8094 | 0.8068 |
| 696                          | 0.8144         | 0.8117 | 0.8091 |
| 698                          | 0.8167         | 0.8141 | 0.8114 |
| 700                          | 0.8190         | 0.8164 | 0.8137 |
| 702                          | 0.8214         | 0.8187 | 0.8161 |
| 704                          | 0.8237         | 0.8211 | 0.8184 |
| 706                          | 0.8261         | 0.8234 | 0.8207 |
| 708                          | 0.8284         | 0.8257 | 0.8230 |
| 710                          | 0.8307         | 0.8281 | 0.8254 |
| 712                          | 0.8331         | 0.8304 | 0.8277 |
| 714                          | 0.8354         | 0.8327 | 0.8300 |
| 716                          | 0.8378         | 0.8350 | 0.8323 |
| 718                          | 0.8401         | 0.8374 | 0.8347 |
| 720                          | 0.8424         | 0.8397 | 0.8370 |
| 722                          | 0.8448         | 0.8420 | 0.8393 |
| 724                          | 0.8471         | 0.8444 | 0.8416 |
| 726                          | 0.8495         | 0.8467 | 0.8440 |
| 728                          | 0.8518         | 0.8490 | 0.8463 |

| Pressure<br>mm of<br>mercury | Temperature °C |        |        |
|------------------------------|----------------|--------|--------|
|                              | 34°            | 35°    | 36°    |
| 730                          | 0.8541         | 0.8514 | 0.8486 |
| 732                          | 0.8565         | 0.8537 | 0.8509 |
| 734                          | 0.8588         | 0.8560 | 0.8533 |
| 736                          | 0.8612         | 0.8584 | 0.8556 |
| 738                          | 0.8635         | 0.8607 | 0.8579 |
| 740                          | 0.8658         | 0.8630 | 0.8602 |
| 742                          | 0.8682         | 0.8654 | 0.8626 |
| 744                          | 0.8705         | 0.8677 | 0.8649 |
| 746                          | 0.8729         | 0.8700 | 0.8672 |
| 748                          | 0.8752         | 0.8724 | 0.8695 |
| 750                          | 0.8775         | 0.8747 | 0.8719 |
| 752                          | 0.8799         | 0.8770 | 0.8742 |
| 754                          | 0.8822         | 0.8794 | 0.8765 |
| 756                          | 0.8846         | 0.8817 | 0.8788 |
| 758                          | 0.8869         | 0.8840 | 0.8812 |
| 760                          | 0.8892         | 0.8864 | 0.8835 |
| 762                          | 0.8916         | 0.8887 | 0.8858 |
| 764                          | 0.8939         | 0.8910 | 0.8881 |
| 766                          | 0.8963         | 0.8934 | 0.8905 |
| 768                          | 0.8986         | 0.8957 | 0.8928 |
| 770                          | 0.9009         | 0.8980 | 0.8951 |
| 772                          | 0.9033         | 0.9004 | 0.8974 |
| 774                          | 0.9056         | 0.9027 | 0.8998 |
| 776                          | 0.9080         | 0.9050 | 0.9021 |
| 778                          | 0.9103         | 0.9074 | 0.9044 |
| 780                          | 0.9127         | 0.9097 | 0.9067 |
| 782                          | 0.9150         | 0.9120 | 0.9091 |
| 784                          | 0.9173         | 0.9144 | 0.9114 |
| 786                          | 0.9197         | 0.9167 | 0.9137 |
| 788                          | 0.9220         | 0.9190 | 0.9160 |

**TABLE 2.20** Values of Absorbance for Percent Absorption

To convert percent absorption (% A) to absorbance, find the present absorption to the nearest whole digit in the left-hand column; read across to the column located under the tenth of a percent desired, and read the value of absorbance. The value of absorbance corresponding to 26.8% absorption is thus 0.1355.

| % A  | .0    | .1    | .2    | .3    | .4    | .5    | .6    | .7    | .8    | .9    |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.0  | .0000 | .0004 | .0009 | .0013 | .0017 | .0022 | .0026 | .0031 | .0035 | .0039 |
| 1.0  | .0044 | .0048 | .0052 | .0057 | .0061 | .0066 | .0070 | .0074 | .0079 | .0083 |
| 2.0  | .0088 | .0092 | .0097 | .0101 | .0106 | .0110 | .0114 | .0119 | .0123 | .0128 |
| 3.0  | .0132 | .0137 | .0141 | .0146 | .0150 | .0155 | .0159 | .0164 | .0168 | .0173 |
| 4.0  | .0177 | .0182 | .0186 | .0191 | .0195 | .0200 | .0205 | .0209 | .0214 | .0218 |
| 5.0  | .0223 | .0227 | .0232 | .0236 | .0241 | .0246 | .0250 | .0255 | .0259 | .0264 |
| 6.0  | .0269 | .0273 | .0278 | .0283 | .0287 | .0292 | .0297 | .0301 | .0306 | .0311 |
| 7.0  | .0315 | .0320 | .0325 | .0329 | .0334 | .0339 | .0343 | .0348 | .0353 | .0357 |
| 8.0  | .0362 | .0367 | .0372 | .0376 | .0381 | .0386 | .0391 | .0395 | .0400 | .0405 |
| 9.0  | .0410 | .0414 | .0419 | .0424 | .0429 | .0434 | .0438 | .0443 | .0448 | .0453 |
| 10.0 | .0458 | .0462 | .0467 | .0472 | .0477 | .0482 | .0487 | .0491 | .0496 | .0501 |
| 11.0 | .0506 | .0511 | .0516 | .0521 | .0526 | .0531 | .0535 | .0540 | .0545 | .0550 |
| 12.0 | .0555 | .0560 | .0565 | .0570 | .0575 | .0580 | .0585 | .0590 | .0595 | .0600 |
| 13.0 | .0605 | .0610 | .0615 | .0620 | .0625 | .0630 | .0635 | .0640 | .0645 | .0650 |
| 14.0 | .0655 | .0660 | .0665 | .0670 | .0675 | .0680 | .0685 | .0691 | .0696 | .0701 |
| 15.0 | .0706 | .0711 | .0716 | .0721 | .0726 | .0731 | .0737 | .0742 | .0747 | .0752 |
| 16.0 | .0757 | .0762 | .0768 | .0773 | .0778 | .0783 | .0788 | .0794 | .0799 | .0804 |
| 17.0 | .0809 | .0814 | .0820 | .0825 | .0830 | .0835 | .0841 | .0846 | .0851 | .0857 |
| 18.0 | .0862 | .0867 | .0872 | .0878 | .0883 | .0888 | .0894 | .0899 | .0904 | .0910 |
| 19.0 | .0915 | .0921 | .0926 | .0931 | .0937 | .0942 | .0947 | .0953 | .0958 | .0964 |
| 20.0 | .0969 | .0975 | .0980 | .0985 | .0991 | .0996 | .1002 | .1007 | .1013 | .1018 |
| 21.0 | .1024 | .1029 | .1035 | .1040 | .1046 | .1051 | .1057 | .1062 | .1068 | .1073 |
| 22.0 | .1079 | .1085 | .1090 | .1096 | .1101 | .1107 | .1113 | .1118 | .1124 | .1129 |
| 23.0 | .1135 | .1141 | .1146 | .1152 | .1158 | .1163 | .1169 | .1175 | .1180 | .1186 |
| 24.0 | .1192 | .1198 | .1203 | .1209 | .1215 | .1221 | .1226 | .1232 | .1238 | .1244 |
| 25.0 | .1249 | .1255 | .1261 | .1267 | .1273 | .1278 | .1284 | .1290 | .1296 | .1302 |
| 26.0 | .1308 | .1314 | .1319 | .1325 | .1331 | .1337 | .1343 | .1349 | .1355 | .1361 |
| 27.0 | .1367 | .1373 | .1379 | .1385 | .1391 | .1397 | .1403 | .1409 | .1415 | .1421 |
| 28.0 | .1427 | .1433 | .1439 | .1445 | .1451 | .1457 | .1463 | .1469 | .1475 | .1481 |
| 29.0 | .1487 | .1494 | .1500 | .1506 | .1512 | .1518 | .1524 | .1530 | .1537 | .1543 |
| 30.0 | .1549 | .1555 | .1561 | .1568 | .1574 | .1580 | .1586 | .1593 | .1599 | .1605 |
| 31.0 | .1612 | .1618 | .1624 | .1630 | .1637 | .1643 | .1649 | .1656 | .1662 | .1669 |
| 32.0 | .1675 | .1681 | .1688 | .1694 | .1701 | .1707 | .1713 | .1720 | .1726 | .1733 |
| 33.0 | .1739 | .1746 | .1752 | .1759 | .1765 | .1772 | .1778 | .1785 | .1791 | .1798 |
| 34.0 | .1805 | .1811 | .1818 | .1824 | .1831 | .1838 | .1844 | .1851 | .1858 | .1864 |
| 35.0 | .1871 | .1878 | .1884 | .1891 | .1898 | .1904 | .1911 | .1918 | .1925 | .1931 |
| 36.0 | .1938 | .1945 | .1952 | .1959 | .1965 | .1972 | .1979 | .1986 | .1993 | .2000 |
| 37.0 | .2007 | .2013 | .2020 | .2027 | .2034 | .2041 | .2048 | .2055 | .2062 | .2069 |
| 38.0 | .2076 | .2083 | .2090 | .2097 | .2104 | .2111 | .2118 | .2125 | .2132 | .2140 |
| 39.0 | .2147 | .2154 | .2161 | .2168 | .2175 | .2182 | .2190 | .2197 | .2204 | .2211 |
| 40.0 | .2218 | .2226 | .2233 | .2240 | .2248 | .2255 | .2262 | .2269 | .2277 | .2284 |
| 41.0 | .2291 | .2299 | .2306 | .2314 | .2321 | .2328 | .2336 | .2343 | .2351 | .2358 |



**TABLE 2.20** Values of Absorbance for Percent Absorption (*Continued*)

| % A  | .0    | .1    | .2    | .3    | .4    | .5    | .6    | .7    | .8    | .9    |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 42.0 | .2366 | .2373 | .2381 | .2388 | .2396 | .2403 | .2411 | .2418 | .2426 | .2434 |
| 43.0 | .2441 | .2449 | .2457 | .2464 | .2472 | .2480 | .2487 | .2495 | .2503 | .2510 |
| 44.0 | .2518 | .2526 | .2534 | .2541 | .2549 | .2557 | .2565 | .2573 | .2581 | .2588 |
| 45.0 | .2596 | .2604 | .2612 | .2620 | .2628 | .2636 | .2644 | .2652 | .2660 | .2668 |
| 46.0 | .2676 | .2684 | .2692 | .2700 | .2708 | .2716 | .2725 | .2733 | .2741 | .2749 |
| 47.0 | .2757 | .2765 | .2774 | .2782 | .2790 | .2798 | .2807 | .2815 | .2823 | .2832 |
| 48.0 | .2840 | .2848 | .2857 | .2865 | .2874 | .2882 | .2890 | .2899 | .2907 | .2916 |
| 49.0 | .2924 | .2933 | .2941 | .2950 | .2958 | .2967 | .2976 | .2984 | .2993 | .3002 |
| 50.0 | .3010 | .3019 | .3028 | .3036 | .3045 | .3054 | .3063 | .3072 | .3080 | .3089 |
| 51.0 | .3098 | .3107 | .3116 | .3125 | .3134 | .3143 | .3152 | .3161 | .3170 | .3179 |
| 52.0 | .3188 | .3197 | .3206 | .3215 | .3224 | .3233 | .3242 | .3251 | .3261 | .3270 |
| 53.0 | .3279 | .3288 | .3298 | .3307 | .3316 | .3325 | .3335 | .3344 | .3354 | .3363 |
| 54.0 | .3372 | .3382 | .3391 | .3401 | .3410 | .3420 | .3429 | .3439 | .3449 | .3458 |
| 55.0 | .3468 | .3478 | .3487 | .3497 | .3507 | .3516 | .3526 | .3536 | .3546 | .3556 |
| 56.0 | .3565 | .3575 | .3585 | .3595 | .3605 | .3615 | .3625 | .3635 | .3645 | .3655 |
| 57.0 | .3665 | .3675 | .3686 | .3696 | .3706 | .3716 | .3726 | .3737 | .3747 | .3757 |
| 58.0 | .3768 | .3778 | .3788 | .3799 | .3809 | .3820 | .3830 | .3840 | .3851 | .3862 |
| 59.0 | .3872 | .3883 | .3893 | .3904 | .3915 | .3925 | .3936 | .3947 | .3958 | .3969 |
| 60.0 | .3979 | .3990 | .4001 | .4012 | .4023 | .4034 | .4045 | .4056 | .4067 | .4078 |
| 61.0 | .4089 | .4101 | .4112 | .4123 | .4134 | .4145 | .4157 | .4168 | .4179 | .4191 |
| 62.0 | .4202 | .4214 | .4225 | .4237 | .4248 | .4260 | .4271 | .4283 | .4295 | .4306 |
| 63.0 | .4318 | .4330 | .4342 | .4353 | .4365 | .4377 | .4389 | .4401 | .4413 | .4425 |
| 64.0 | .4437 | .4449 | .4461 | .4473 | .4485 | .4498 | .4510 | .4522 | .4535 | .4547 |
| 65.0 | .4559 | .4572 | .4584 | .4597 | .4609 | .4622 | .4634 | .4647 | .4660 | .4672 |
| 66.0 | .4685 | .4698 | .4711 | .4724 | .4737 | .4750 | .4763 | .4776 | .4789 | .4802 |
| 67.0 | .4815 | .4828 | .4841 | .4855 | .4868 | .4881 | .4895 | .4908 | .4921 | .4935 |
| 68.0 | .4948 | .4962 | .4976 | .4989 | .5003 | .5017 | .5031 | .5045 | .5058 | .5072 |
| 69.0 | .5086 | .5100 | .5114 | .5129 | .5143 | .5157 | .5171 | .5186 | .5200 | .5214 |
| 70.0 | .5229 | .5243 | .5258 | .5272 | .5287 | .5302 | .5317 | .5331 | .5346 | .5361 |
| 71.0 | .5376 | .5391 | .5406 | .5421 | .5436 | .5452 | .5467 | .5482 | .5498 | .5513 |
| 72.0 | .5528 | .5544 | .5560 | .5575 | .5591 | .5607 | .5622 | .5638 | .5654 | .5670 |
| 73.0 | .5686 | .5702 | .5719 | .5735 | .5751 | .5768 | .5784 | .5800 | .5817 | .5834 |
| 74.0 | .5850 | .5867 | .5884 | .5901 | .5918 | .5935 | .5952 | .5969 | .5986 | .6003 |
| 75.0 | .6021 | .6038 | .6055 | .6073 | .6091 | .6108 | .6126 | .6144 | .6162 | .6180 |
| 76.0 | .6198 | .6216 | .6234 | .6253 | .6271 | .6289 | .6308 | .6326 | .6345 | .6364 |
| 77.0 | .6383 | .6402 | .6421 | .6440 | .6459 | .6478 | .6498 | .6517 | .6536 | .6556 |
| 78.0 | .6576 | .6596 | .6615 | .6635 | .6655 | .6676 | .6696 | .6716 | .6737 | .6757 |
| 79.0 | .6778 | .6799 | .6819 | .6840 | .6861 | .6882 | .6904 | .6925 | .6946 | .6968 |
| 80.0 | .6990 | .7011 | .7033 | .7055 | .7077 | .7100 | .7122 | .7144 | .7167 | .7190 |
| 81.0 | .7212 | .7235 | .7258 | .7282 | .7305 | .7328 | .7352 | .7375 | .7399 | .7423 |
| 82.0 | .7447 | .7471 | .7496 | .7520 | .7545 | .7570 | .7595 | .7620 | .7645 | .7670 |
| 83.0 | .7696 | .7721 | .7747 | .7773 | .7799 | .7825 | .7852 | .7878 | .7905 | .7932 |
| 84.0 | .7959 | .7986 | .8013 | .8041 | .8069 | .8097 | .8125 | .8153 | .8182 | .8210 |
| 85.0 | .8239 | .8268 | .8297 | .8327 | .8356 | .8386 | .8416 | .8447 | .8477 | .8508 |
| 86.0 | .8539 | .8570 | .8601 | .8633 | .8665 | .8697 | .8729 | .8761 | .8794 | .8827 |
| 87.0 | .8861 | .8894 | .8928 | .8962 | .8996 | .9031 | .9066 | .9101 | .9136 | .9172 |
| 88.0 | .9208 | .9245 | .9281 | .9318 | .9355 | .9393 | .9431 | .9469 | .9508 | .9547 |
| 89.0 | .9586 | .9626 | .9666 | .9706 | .9747 | .9788 | .9830 | .9872 | .9914 | .9957 |

**TABLE 2.21** Transmittance-Absorbance Conversion Table

*From Meites, Handbook of Analytical Chemistry, 1963, McGraw-Hill Book Company; by permission.*

This table gives absorbance values to four significant figures corresponding to % transmittance values which are given to three significant figures. The values of % transmittance are given in the left-hand column and in the top row. For example, 8.4% transmittance corresponds to an absorbance of 1.076.

Interpolation is facilitated and accuracy is maximized if the % transmittance is between 1 and 10, by multiplying its value by 10, finding the absorbance corresponding to the result, and adding 1. For example, to find the absorbance corresponding to 8.45% transmittance, note that 84.5% transmittance corresponds to an absorbance of 0.0731, so that 8.45% transmittance corresponds to an absorbance of 1.0731. For % transmittance values between 0.1 and 1, multiply by 100, find the absorbance corresponding to the result, and add 2.

Conversely, to find the % transmittance corresponding to an absorbance between 1 and 2, subtract 1 from the absorbance, find the % transmittance corresponding to the result, and divide by 10. For example, an absorbance of 1.219 can best be converted to % transmittance by noting that an absorbance of 0.219 would correspond to 60.4% transmittance; dividing this by 10 gives the desired value, 6.04% transmittance. For absorbance values between 2 and 3, subtract 2 from the absorbance, find the % transmittance corresponding to the result, and divide by 100.

| % Transmittance | 0.0    | 0.1    | 0.2    | 0.3    | 0.4    | 0.5    | 0.6    | 0.7    | 0.8    | 0.9    |
|-----------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 0               | .....  | 3.000  | 2.699  | 2.523  | 2.398  | 2.301  | 2.222  | 2.155  | 2.097  | 2.046  |
| 1               | 2.000  | 1.959  | 1.921  | 1.886  | 1.854  | 1.824  | 1.796  | 1.770  | 1.745  | 1.721  |
| 2               | 1.699  | 1.678  | 1.658  | 1.638  | 1.620  | 1.602  | 1.585  | 1.569  | 1.553  | 1.538  |
| 3               | 1.523  | 1.509  | 1.495  | 1.481  | 1.469  | 1.456  | 1.444  | 1.432  | 1.420  | 1.409  |
| 4               | 1.398  | 1.387  | 1.377  | 1.367  | 1.357  | 1.347  | 1.337  | 1.328  | 1.319  | 1.310  |
| 5               | 1.301  | 1.292  | 1.284  | 1.276  | 1.268  | 1.260  | 1.252  | 1.244  | 1.237  | 1.229  |
| 6               | 1.222  | 1.215  | 1.208  | 1.201  | 1.194  | 1.187  | 1.180  | 1.174  | 1.167  | 1.161  |
| 7               | 1.155  | 1.149  | 1.143  | 1.137  | 1.131  | 1.125  | 1.119  | 1.114  | 1.108  | 1.102  |
| 8               | 1.097  | 1.092  | 1.086  | 1.081  | 1.076  | 1.071  | 1.066  | 1.060  | 1.056  | 1.051  |
| 9               | 1.046  | 1.041  | 1.036  | 1.032  | 1.027  | 1.022  | 1.018  | 1.013  | 1.009  | 1.004  |
| 10              | 1.000  | 0.9957 | 0.9914 | 0.9872 | 0.9830 | 0.9788 | 0.9747 | 0.9706 | 0.9666 | 0.9626 |
| 11              | 0.9586 | 0.9547 | 0.9508 | 0.9469 | 0.9431 | 0.9393 | 0.9355 | 0.9318 | 0.9281 | 0.9245 |
| 12              | 0.9208 | 0.9172 | 0.9136 | 0.9101 | 0.9066 | 0.9031 | 0.8996 | 0.8962 | 0.8928 | 0.8894 |
| 13              | 0.8861 | 0.8827 | 0.8794 | 0.8761 | 0.8729 | 0.8697 | 0.8665 | 0.8633 | 0.8601 | 0.8570 |
| 14              | 0.8539 | 0.8508 | 0.8477 | 0.8447 | 0.8416 | 0.8386 | 0.8356 | 0.8327 | 0.8297 | 0.8268 |
| 15              | 0.8239 | 0.8210 | 0.8182 | 0.8153 | 0.8125 | 0.8097 | 0.8069 | 0.8041 | 0.8013 | 0.7986 |
| 16              | 0.7959 | 0.7932 | 0.7905 | 0.7878 | 0.7852 | 0.7825 | 0.7799 | 0.7773 | 0.7747 | 0.7721 |
| 17              | 0.7696 | 0.7670 | 0.7645 | 0.7620 | 0.7595 | 0.7570 | 0.7545 | 0.7520 | 0.7496 | 0.7471 |
| 18              | 0.7447 | 0.7423 | 0.7399 | 0.7375 | 0.7352 | 0.7328 | 0.7305 | 0.7282 | 0.7258 | 0.7235 |
| 19              | 0.7212 | 0.7190 | 0.7167 | 0.7144 | 0.7122 | 0.7100 | 0.7077 | 0.7055 | 0.7033 | 0.7011 |
| 20              | 0.6990 | 0.6968 | 0.6946 | 0.6925 | 0.6904 | 0.6882 | 0.6861 | 0.6840 | 0.6819 | 0.6799 |
| 21              | 0.6778 | 0.6757 | 0.6737 | 0.6716 | 0.6696 | 0.6676 | 0.6655 | 0.6635 | 0.6615 | 0.6596 |
| 22              | 0.6576 | 0.6556 | 0.6536 | 0.6517 | 0.6498 | 0.6478 | 0.6459 | 0.6440 | 0.6421 | 0.6402 |
| 23              | 0.6383 | 0.6364 | 0.6345 | 0.6326 | 0.6308 | 0.6289 | 0.6271 | 0.6253 | 0.6234 | 0.6216 |
| 24              | 0.6198 | 0.6180 | 0.6162 | 0.6144 | 0.6126 | 0.6108 | 0.6091 | 0.6073 | 0.6055 | 0.6038 |
| 25              | 0.6021 | 0.6003 | 0.5986 | 0.5969 | 0.5952 | 0.5935 | 0.5918 | 0.5901 | 0.5884 | 0.5867 |
| 26              | 0.5850 | 0.5834 | 0.5817 | 0.5800 | 0.5784 | 0.5766 | 0.5751 | 0.5735 | 0.5719 | 0.5702 |
| 27              | 0.5686 | 0.5670 | 0.5654 | 0.5638 | 0.5622 | 0.5607 | 0.5591 | 0.5575 | 0.5560 | 0.5544 |
| 28              | 0.5528 | 0.5513 | 0.5498 | 0.5482 | 0.5467 | 0.5452 | 0.5436 | 0.5421 | 0.5406 | 0.5391 |
| 29              | 0.5376 | 0.5361 | 0.5346 | 0.5331 | 0.5317 | 0.5302 | 0.5287 | 0.5272 | 0.5258 | 0.5243 |
| 30              | 0.5229 | 0.5214 | 0.5200 | 0.5186 | 0.5171 | 0.5157 | 0.5143 | 0.5129 | 0.5114 | 0.5100 |

**TABLE 2.21** Transmittance-Absorbance Conversion Table (*Continued*)

| %<br>Trans-<br>mittance | 0.0    | 0.1    | 0.2    | 0.3    | 0.4    | 0.5    | 0.6    | 0.7    | 0.8    | 0.9    |
|-------------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 31                      | 0.5086 | 0.5072 | 0.5058 | 0.5045 | 0.5031 | 0.5017 | 0.5003 | 0.4989 | 0.4976 | 0.4962 |
| 32                      | 0.4949 | 0.4935 | 0.4921 | 0.4908 | 0.4895 | 0.4881 | 0.4868 | 0.4855 | 0.4841 | 0.4828 |
| 33                      | 0.4815 | 0.4802 | 0.4789 | 0.4776 | 0.4763 | 0.4750 | 0.4737 | 0.4724 | 0.4711 | 0.4698 |
| 34                      | 0.4685 | 0.4672 | 0.4660 | 0.4647 | 0.4634 | 0.4622 | 0.4609 | 0.4597 | 0.4584 | 0.4572 |
| 35                      | 0.4559 | 0.4547 | 0.4535 | 0.4522 | 0.4510 | 0.4498 | 0.4486 | 0.4473 | 0.4461 | 0.4449 |
| 36                      | 0.4437 | 0.4425 | 0.4413 | 0.4401 | 0.4389 | 0.4377 | 0.4365 | 0.4353 | 0.4342 | 0.4330 |
| 37                      | 0.4318 | 0.4306 | 0.4295 | 0.4283 | 0.4271 | 0.4260 | 0.4248 | 0.4237 | 0.4225 | 0.4214 |
| 38                      | 0.4202 | 0.4191 | 0.4179 | 0.4168 | 0.4157 | 0.4145 | 0.4134 | 0.4123 | 0.4112 | 0.4101 |
| 39                      | 0.4089 | 0.4078 | 0.4067 | 0.4056 | 0.4045 | 0.4034 | 0.4023 | 0.4012 | 0.4001 | 0.3989 |
| 40                      | 0.3979 | 0.3969 | 0.3958 | 0.3947 | 0.3936 | 0.3925 | 0.3915 | 0.3904 | 0.3893 | 0.3883 |
| 41                      | 0.3872 | 0.3862 | 0.3851 | 0.3840 | 0.3830 | 0.3820 | 0.3809 | 0.3799 | 0.3788 | 0.3778 |
| 42                      | 0.3768 | 0.3757 | 0.3747 | 0.3737 | 0.3726 | 0.3716 | 0.3706 | 0.3696 | 0.3686 | 0.3675 |
| 43                      | 0.3665 | 0.3655 | 0.3645 | 0.3635 | 0.3625 | 0.3615 | 0.3605 | 0.3595 | 0.3585 | 0.3575 |
| 44                      | 0.3565 | 0.3556 | 0.3546 | 0.3536 | 0.3526 | 0.3516 | 0.3507 | 0.3497 | 0.3487 | 0.3478 |
| 45                      | 0.3468 | 0.3458 | 0.3449 | 0.3439 | 0.3429 | 0.3420 | 0.3410 | 0.3401 | 0.3391 | 0.3382 |
| 46                      | 0.3372 | 0.3363 | 0.3354 | 0.3344 | 0.3335 | 0.3325 | 0.3316 | 0.3307 | 0.3298 | 0.3288 |
| 47                      | 0.3279 | 0.3270 | 0.3261 | 0.3251 | 0.3242 | 0.3233 | 0.3224 | 0.3215 | 0.3206 | 0.3197 |
| 48                      | 0.3188 | 0.3179 | 0.3170 | 0.3161 | 0.3152 | 0.3143 | 0.3134 | 0.3125 | 0.3116 | 0.3107 |
| 49                      | 0.3098 | 0.3089 | 0.3080 | 0.3072 | 0.3063 | 0.3054 | 0.3045 | 0.3036 | 0.3028 | 0.3019 |
| 50                      | 0.3010 | 0.3002 | 0.2993 | 0.2984 | 0.2976 | 0.2967 | 0.2958 | 0.2950 | 0.2941 | 0.2933 |
| 51                      | 0.2924 | 0.2916 | 0.2907 | 0.2899 | 0.2890 | 0.2882 | 0.2874 | 0.2865 | 0.2857 | 0.2848 |
| 52                      | 0.2840 | 0.2832 | 0.2823 | 0.2815 | 0.2807 | 0.2798 | 0.2790 | 0.2782 | 0.2774 | 0.2765 |
| 53                      | 0.2757 | 0.2749 | 0.2741 | 0.2733 | 0.2725 | 0.2716 | 0.2708 | 0.2700 | 0.2692 | 0.2684 |
| 54                      | 0.2676 | 0.2668 | 0.2660 | 0.2652 | 0.2644 | 0.2636 | 0.2628 | 0.2620 | 0.2612 | 0.2604 |
| 55                      | 0.2596 | 0.2588 | 0.2581 | 0.2573 | 0.2565 | 0.2557 | 0.2549 | 0.2541 | 0.2534 | 0.2526 |
| 56                      | 0.2518 | 0.2510 | 0.2503 | 0.2495 | 0.2487 | 0.2480 | 0.2472 | 0.2464 | 0.2457 | 0.2449 |
| 57                      | 0.2441 | 0.2434 | 0.2426 | 0.2418 | 0.2411 | 0.2403 | 0.2396 | 0.2388 | 0.2381 | 0.2373 |
| 58                      | 0.2366 | 0.2358 | 0.2351 | 0.2343 | 0.2336 | 0.2328 | 0.2321 | 0.2314 | 0.2306 | 0.2299 |
| 59                      | 0.2291 | 0.2284 | 0.2277 | 0.2269 | 0.2262 | 0.2255 | 0.2248 | 0.2240 | 0.2233 | 0.2226 |
| 60                      | 0.2218 | 0.2211 | 0.2204 | 0.2197 | 0.2190 | 0.2182 | 0.2175 | 0.2168 | 0.2161 | 0.2154 |
| 61                      | 0.2147 | 0.2140 | 0.2132 | 0.2125 | 0.2118 | 0.2111 | 0.2104 | 0.2097 | 0.2090 | 0.2083 |
| 62                      | 0.2076 | 0.2069 | 0.2062 | 0.2055 | 0.2048 | 0.2041 | 0.2034 | 0.2027 | 0.2020 | 0.2013 |
| 63                      | 0.2007 | 0.2000 | 0.1993 | 0.1986 | 0.1979 | 0.1972 | 0.1965 | 0.1959 | 0.1952 | 0.1945 |
| 64                      | 0.1938 | 0.1931 | 0.1925 | 0.1918 | 0.1911 | 0.1904 | 0.1898 | 0.1891 | 0.1884 | 0.1878 |
| 65                      | 0.1871 | 0.1864 | 0.1858 | 0.1851 | 0.1844 | 0.1838 | 0.1831 | 0.1824 | 0.1818 | 0.1811 |
| 66                      | 0.1805 | 0.1798 | 0.1791 | 0.1785 | 0.1778 | 0.1772 | 0.1765 | 0.1759 | 0.1752 | 0.1746 |
| 67                      | 0.1739 | 0.1733 | 0.1726 | 0.1720 | 0.1713 | 0.1707 | 0.1701 | 0.1694 | 0.1688 | 0.1681 |
| 68                      | 0.1675 | 0.1669 | 0.1662 | 0.1656 | 0.1649 | 0.1643 | 0.1637 | 0.1630 | 0.1624 | 0.1618 |
| 69                      | 0.1612 | 0.1605 | 0.1599 | 0.1593 | 0.1586 | 0.1580 | 0.1574 | 0.1568 | 0.1561 | 0.1555 |
| 70                      | 0.1549 | 0.1543 | 0.1537 | 0.1530 | 0.1524 | 0.1518 | 0.1512 | 0.1506 | 0.1500 | 0.1494 |
| 71                      | 0.1487 | 0.1481 | 0.1475 | 0.1469 | 0.1463 | 0.1457 | 0.1451 | 0.1445 | 0.1439 | 0.1433 |
| 72                      | 0.1427 | 0.1421 | 0.1415 | 0.1409 | 0.1403 | 0.1397 | 0.1391 | 0.1385 | 0.1379 | 0.1373 |
| 73                      | 0.1367 | 0.1361 | 0.1355 | 0.1349 | 0.1343 | 0.1337 | 0.1331 | 0.1325 | 0.1319 | 0.1314 |

TABLE 2.21 Transmittance-Absorbance Conversion Table (Continued)

| %<br>Trans-<br>mittance | 0.0    | 0.1    | 0.2    | 0.3    | 0.4    | 0.5    | 0.6    | 0.7    | 0.8    | 0.9    |
|-------------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 74                      | 0.1308 | 0.1302 | 0.1296 | 0.1290 | 0.1284 | 0.1278 | 0.1273 | 0.1267 | 0.1261 | 0.1255 |
| 75                      | 0.1249 | 0.1244 | 0.1238 | 0.1232 | 0.1226 | 0.1221 | 0.1215 | 0.1209 | 0.1203 | 0.1198 |
| 76                      | 0.1192 | 0.1186 | 0.1180 | 0.1175 | 0.1169 | 0.1163 | 0.1158 | 0.1152 | 0.1146 | 0.1141 |
| 77                      | 0.1135 | 0.1129 | 0.1124 | 0.1118 | 0.1113 | 0.1107 | 0.1101 | 0.1096 | 0.1090 | 0.1085 |
| 78                      | 0.1079 | 0.1073 | 0.1068 | 0.1062 | 0.1057 | 0.1051 | 0.1046 | 0.1040 | 0.1035 | 0.1029 |
| 79                      | 0.1024 | 0.1018 | 0.1013 | 0.1007 | 0.1002 | 0.0996 | 0.0991 | 0.0985 | 0.0980 | 0.0975 |
| 80                      | 0.0969 | 0.0964 | 0.0958 | 0.0953 | 0.0947 | 0.0942 | 0.0937 | 0.0931 | 0.0926 | 0.0921 |
| 81                      | 0.0915 | 0.0910 | 0.0904 | 0.0899 | 0.0894 | 0.0888 | 0.0883 | 0.0878 | 0.0872 | 0.0867 |
| 82                      | 0.0862 | 0.0857 | 0.0851 | 0.0846 | 0.0841 | 0.0835 | 0.0830 | 0.0825 | 0.0820 | 0.0814 |
| 83                      | 0.0809 | 0.0804 | 0.0799 | 0.0794 | 0.0788 | 0.0783 | 0.0778 | 0.0773 | 0.0768 | 0.0762 |
| 84                      | 0.0757 | 0.0752 | 0.0747 | 0.0742 | 0.0737 | 0.0731 | 0.0726 | 0.0721 | 0.0716 | 0.0711 |
| 85                      | 0.0706 | 0.0701 | 0.0696 | 0.0691 | 0.0685 | 0.0680 | 0.0675 | 0.0670 | 0.0665 | 0.0660 |
| 86                      | 0.0655 | 0.0650 | 0.0645 | 0.0640 | 0.0635 | 0.0630 | 0.0625 | 0.0620 | 0.0615 | 0.0610 |
| 87                      | 0.0605 | 0.0600 | 0.0595 | 0.0590 | 0.0585 | 0.0580 | 0.0575 | 0.0570 | 0.0565 | 0.0560 |
| 88                      | 0.0555 | 0.0550 | 0.0545 | 0.0540 | 0.0535 | 0.0531 | 0.0526 | 0.0521 | 0.0516 | 0.0511 |
| 89                      | 0.0506 | 0.0501 | 0.0496 | 0.0491 | 0.0487 | 0.0482 | 0.0477 | 0.0472 | 0.0467 | 0.0462 |
| 90                      | 0.0458 | 0.0453 | 0.0448 | 0.0443 | 0.0438 | 0.0434 | 0.0429 | 0.0424 | 0.0419 | 0.0414 |
| 91                      | 0.0410 | 0.0405 | 0.0400 | 0.0395 | 0.0391 | 0.0386 | 0.0381 | 0.0376 | 0.0372 | 0.0367 |
| 92                      | 0.0362 | 0.0357 | 0.0353 | 0.0348 | 0.0343 | 0.0339 | 0.0334 | 0.0329 | 0.0325 | 0.0320 |
| 93                      | 0.0315 | 0.0311 | 0.0306 | 0.0301 | 0.0297 | 0.0292 | 0.0287 | 0.0283 | 0.0278 | 0.0273 |
| 94                      | 0.0269 | 0.0264 | 0.0259 | 0.0255 | 0.0250 | 0.0246 | 0.0241 | 0.0237 | 0.0232 | 0.0227 |
| 95                      | 0.0223 | 0.0218 | 0.0214 | 0.0209 | 0.0205 | 0.0200 | 0.0195 | 0.0191 | 0.0186 | 0.0182 |
| 96                      | 0.0177 | 0.0173 | 0.0168 | 0.0164 | 0.0159 | 0.0155 | 0.0150 | 0.0146 | 0.0141 | 0.0137 |
| 97                      | 0.0132 | 0.0128 | 0.0123 | 0.0119 | 0.0114 | 0.0110 | 0.0106 | 0.0101 | 0.0097 | 0.0092 |
| 98                      | 0.0088 | 0.0083 | 0.0079 | 0.0074 | 0.0070 | 0.0066 | 0.0061 | 0.0057 | 0.0052 | 0.0048 |
| 99                      | 0.0044 | 0.0039 | 0.0035 | 0.0031 | 0.0026 | 0.0022 | 0.0017 | 0.0013 | 0.0009 | 0.0004 |



## 2.2 MATHEMATICAL TABLES

---

### 2.2.1 Logarithms

#### 2.2.1.1 Properties and Uses

*Definition of Logarithm.* The *logarithm*  $x$  of the number  $N$  to the base  $b$  is the exponent of the power to which  $b$  must be raised to give  $N$ . That is,

$$\log_b N = x \quad \text{or} \quad b^x = N$$

The number  $N$  is positive and  $b$  may be any positive number except 1.

*Properties of Logarithms*

1. The logarithm of a product is equal to the sum of the logarithms of the factors; thus,

$$\log_b M \cdot N = \log_b M + \log_b N$$

2. The logarithm of a quotient is equal to the logarithm of the numerator minus the logarithm of the denominator; thus,

$$\log_b \frac{M}{N} = \log_b M - \log_b N$$

3. The logarithm of a power of a number is equal to the logarithm of the base multiplied by the exponent of the power; thus,

$$\log_b M^p = p \cdot \log_b M$$

4. The logarithm of a root of a number is equal to the logarithm of the number divided by the index of the root; thus

$$\log_b \sqrt[q]{M} = \frac{1}{q} \log_b M$$

Other properties of logarithms:

$$\log_b b = 1 \quad \log_b \sqrt[q]{M^p} = \frac{p}{q} \log_b M$$

$$\log_b 1 = 0 \quad \log_b N = \log_a N \cdot \log_b a = \frac{\log_a N}{\log_a b}$$

$$\log_b (b^N) = N \quad b^{\log_b N} = N$$

*Systems of Logarithms.* There are two common systems of logarithms in use: (1) the *natural* (Napierian or hyperbolic) system which uses the base  $e = 2.71828 \dots$ ; (2) the *common* (Briggsian) system which uses the base 10.

We shall use the abbreviation  $\log N \equiv \log_{10} N$  in this section.

Unless otherwise stated, tables of logarithms are always tables of common logarithms.

*Characteristic of a Common Logarithm of a Number.* Every real positive number has a real common logarithm such that if  $a < b$ ,  $\log a < \log b$ . Neither zero nor any negative number has a real logarithm.

A common logarithm, in general, consists of an integer, which is called the *characteristic*, and a decimal (usually endless), which is called the *mantissa*. The characteristic of any number may be determined from the following rules:

*Rule I.* The characteristic of any number greater than 1 is one less than the number of digits before the decimal point.

*Rule II.\** The characteristic of a number less than 1 is found by subtracting from 9 the number of ciphers between the decimal point and the first significant digit, and writing  $-10$  after the result.

Thus the characteristic of  $\log 936$  is 2; the characteristic of  $\log 9.36$  is 0; of  $\log 0.936$  is  $9 - 10$ ; of  $\log 0.00936$  is  $7 - 10$ .

*Mantissa of a Common Logarithm of a Number.* An important consequence of the use of base 10 is that the mantissa of a number is independent of the position of the decimal point. Thus 93 600, 93.600, 0.000 936, all have the same mantissa. Hence in Tables of Common Logarithms only mantissas are given. A five-place table gives the values of the mantissa correct to five places of decimals.

Since it is possible to obtain logarithms by using hand calculators, this Handbook contains no logarithm tables.

#### *Helpful Hints*

1. When connecting numbers to logarithms, use as many decimal places in the mantissa as there are significant digits in the number.
2. When finding the antilogarithm, keep as many significant digits as there are decimal places in the mantissa.

*Examples:*  $\log 10.35 = 1.0149$ ;  $\text{antilog } 0.065 = 1.16$ .

---

\* Some writers use a dash over the characteristic to indicate a negative value; for example,

$$\log 0.004657 = 7.6681 - 10 = \bar{3}.6681$$

**TABLE 2.23** Derivatives and Differentiation*Rules for differentiation.*

From Baumeister and Marks, *Standard Handbook for Mechanical Engineers*, 7th ed., McGraw-Hill Book Company, New York (1967); by permission.

To find the derivative of a given function at a given point: (1) If the function is given only by a curve, measure graphically the slope of the tangent at the point in question; (2) if the function is given by a mathematical expression, use the following rules for differentiation. These rules give, directly, the differential,  $dy$ , in terms of  $dx$ ; to find the derivative,  $dy/dx$ , divide through by  $dx$ .

Here  $u, v, w, \dots$  represents any functions of a variable  $x$ , or may themselves be independent variables.  $a$  is a constant which does not change in values in the same discussion;  $e = 2.71828$ .

1.  $d(a + u) = du$

2.  $d(au) = a du$

3.  $d(u + v + w + \dots) = du + dv + dw + \dots$

4.  $d(uv) = u dv + v du$

5.  $d(uvw \dots) = (uvw \dots) \left( \frac{du}{u} + \frac{dv}{v} + \frac{dw}{w} + \dots \right)$

6.  $\frac{d}{dv} \frac{u}{v} = \frac{v du - u dv}{v^2}$

7.  $d(u^m) = mu^{m-1} du$

Thus,  $d(u^2) = 2u du$ ;  $d(u^3) = 3u^2 du$ ; etc.

8.  $d\sqrt{u} = \frac{du}{2\sqrt{u}}$

9.  $d\left(\frac{1}{u}\right) = -\frac{du}{u^2}$

10.  $d(e^u) = e^u du$

11.  $d(a^u) = (\ln a)a^u du$

12.  $d \ln u = \frac{du}{u}$

13.  $d \log_{10} u = (\log_{10} e) \frac{du}{u} = (0.4343 \dots) \frac{du}{u}$

14.  $d \sin u = \cos u du$

15.  $d \csc u = -\cot u \csc u du$

16.  $d \cos u = -\sin u du$

17.  $d \sec u = \tan u \sec u du$

18.  $d \tan u = \sec^2 u du$

19.  $d \cot u = -\csc^2 u du$

20.  $d \sin^{-1} u = \frac{du}{\sqrt{1-u^2}}$

21.  $d \csc^{-1} u = -\frac{du}{u\sqrt{u^2-1}}$

22.  $d \cos^{-1} u = -\frac{du}{\sqrt{1-u^2}}$

23.  $d \sec^{-1} u = \frac{du}{u\sqrt{u^2-1}}$

24.  $d \tan^{-1} u = \frac{du}{1+u^2}$

25.  $d \cot^{-1} u = -\frac{du}{1+u^2}$

26.  $d \ln \sin u = \cot u du$

27.  $d \ln \tan u = \frac{2 du}{\sin 2u}$

28.  $d \ln \cos u = -\tan u du$

29.  $d \ln \cot u = -\frac{2 du}{\sin 2u}$

30.  $d \sinh u = \cosh u du$

31.  $d \operatorname{csch} u = -\operatorname{csch} u \coth u du$

32.  $d \cosh u = \sinh u du$

33.  $d \operatorname{sech} u = -\operatorname{sech} u \tanh u du$

34.  $d \tanh u = \operatorname{sech}^2 u du$

35.  $d \coth u = -\operatorname{csch}^2 u du$

36.  $d \sinh^{-1} u = \frac{du}{\sqrt{u^2+1}}$

37.  $d \operatorname{csch}^{-1} u = -\frac{du}{u\sqrt{u^2+1}}$

38.  $d \cosh^{-1} u = \frac{du}{\sqrt{u^2-1}}$

39.  $d \operatorname{sech}^{-1} u = -\frac{du}{u\sqrt{1-u^2}}$

40.  $d \tanh^{-1} u = \frac{du}{1-u^2}$

41.  $d \coth^{-1} u = \frac{du}{1-u^2}$

42.  $d(u^v) = (u^{v-1})(u \ln u dv + v du)$



**TABLE 2.24** Integrals

From *Baumeister and Marks, Standard Handbook for Mechanical Engineers, 7th ed., McGraw-Hill Book Company, New York (1967); by permission.*

An integral of  $f(x) dx$  is any function whose differential is  $f(x) dx$ , and is denoted by  $\int f(x) dx$ . All the integrals of  $f(x) dx$  are included in the expression  $\int f(x) dx + C$ , where  $\int f(x) dx$  is any particular integral, and  $C$  is an arbitrary constant. The process of finding (when possible) an integral of a given function consists in recognizing by inspection a function which, when differentiated, will produce the given function; or in transforming the given function into a form in which such recognition is easy. The most common integrable forms are collected in the following brief table; for a more extended list, see Peirce, *Table of Integrals*, Ginn, or Dwight, *Table of Integrals and other Mathematical Data*, Macmillan.

## General formulas

1.  $\int a du = a \int du = au + C$
2.  $\int (u + v) dx = \int u dx + \int v dx$
3.  $\int u dv = uv - \int v du$
4.  $\int f(x) dx = \int f[F(y)]F'(y) dy, x = F(y)$
5.  $\int dy \int f(x, y) dx = \int dx \int f(x, y) dy$

## Fundamental integrals

6.  $\int x^n dx = \frac{x^{n+1}}{n+1} + C$ , when  $n \neq -1$
7.  $\int \frac{dx}{x} = \ln x + C = \ln cx$
8.  $\int e^x dx = e^x + C$
9.  $\int \sin x dx = -\cos x + C$
10.  $\int \cos x dx = \sin x + C$
11.  $\int \frac{dx}{\sin^2 x} = -\cot x + C$
12.  $\int \frac{dx}{\cos^2 x} = \tan x + C$
13.  $\int \frac{dx}{\sqrt{1-x^2}} = \sin^{-1} x + C = -\cos^{-1} x + C$
14.  $\int \frac{dx}{1+x^2} = \tan^{-1} x + C = -\cot^{-1} x + C$

## Rational functions

15.  $\int (a + bx)^n dx = \frac{(a + bx)^{n+1}}{(n+1)b} + C$
  16.  $\int \frac{dx}{a + bx} = \frac{1}{b} \ln(a + bx) + C = \frac{1}{b} \ln c(a + bx)$
  17.  $\int \frac{1}{x^2} dx = -\frac{1}{x} + C$
  18.  $\int \frac{dx}{(a + bx)^2} = -\frac{1}{b(a + bx)} + C$
  19.  $\int \frac{dx}{1-x^2} = \frac{1}{2} \ln \frac{1+x}{1-x} + C = \tanh^{-1} x + C$ , when  $x < 1$
  20.  $\int \frac{dx}{x^2 - 1} = \frac{1}{2} \ln \frac{x-1}{x+1} + C = -\coth^{-1} x + C$ , when  $x > 1$
  21.  $\int \frac{dx}{a + bx^2} = \frac{1}{\sqrt{ab}} \tan^{-1} \left( \sqrt{\frac{b}{a}} x \right) + C$
  22.  $\int \frac{dx}{a - bx^2} = \frac{1}{2\sqrt{ab}} \ln \frac{\sqrt{ab} + bx}{\sqrt{ab} - bx} + C$
- $\left. \begin{aligned} &= \frac{1}{\sqrt{ab}} \tanh^{-1} \left( \sqrt{\frac{b}{a}} x \right) + C \end{aligned} \right\} [a > 0, b > 0]$

**TABLE 2.24** Integrals (Continued)Rational functions (*continued*)

23. 
$$\int \frac{dx}{a + 2bx + cx^2} = \frac{1}{\sqrt{ac - b^2}} \tan^{-1} \frac{b + cx}{\sqrt{ac - b^2}} + C \left\{ [ac - b^2 > 0] \right.$$
- $$= \frac{1}{2\sqrt{b^2 - ac}} \ln \frac{\sqrt{b^2 - ac} - b - cx}{\sqrt{b^2 - ac} + b + cx} + C$$
- $$= -\frac{1}{\sqrt{b^2 - ac}} \tanh^{-1} \frac{b + cx}{\sqrt{b^2 - ac}} + C \left. \right\} [b^2 - ac > 0]$$
24. 
$$\int \frac{dx}{a + 2bx + cx^2} = -\frac{1}{b + cx} + C, \text{ when } b^2 = ac$$
25. 
$$\int \frac{(m + nx) dx}{a + 2bx + cx^2} = \frac{n}{2c} \ln(a + 2bx + cx^2) + \frac{mc - nb}{c} \int \frac{dx}{a + 2bx + cx^2}$$
26. In  $\int \frac{f(x) dx}{a + 2bx + cx^2}$ , if  $f(x)$  is a polynomial of higher than the first degree, divide by the denominator before integrating.
27. 
$$\int \frac{dx}{(a + 2bx + cx^2)^p} = \frac{1}{2(ac - b^2)(p - 1)} \times \frac{b + cx}{(a + 2bx + cx^2)^{p-1}}$$

$$+ \frac{(2p - 3)c}{2(ac - b^2)(p - 1)} \int \frac{dx}{(a + 2bx + cx^2)^{p-1}}$$
28. 
$$\int \frac{(m + nx) dx}{(a + 2bx + cx^2)^p} = -\frac{n}{2c(p - 1)} \times \frac{1}{(a + 2bx + cx^2)^{p-1}}$$

$$+ \frac{mc - nb}{c} \int \frac{dx}{(a + 2bx + cx^2)^p}$$
29. 
$$\int x^{m-1}(a + bx)^n dx = \frac{x^{m-1}(a + bx)^{n+1}}{(m + n)b} - \frac{(m - 1)a}{(m + n)b} \int x^{m-2}(a + bx)^n dx$$

$$= \frac{x^m(a + bx)^n}{m + n} + \frac{na}{m + n} \int x^{m-1}(a + bx)^{n-1} dx$$

## Irrational functions

30. 
$$\int \sqrt{a + bx} dx = \frac{2}{3b} \sqrt{(a + bx)^3} + C$$
31. 
$$\int \frac{dx}{\sqrt{a + bx}} = \frac{2}{b} \sqrt{a + bx} + C$$
32. 
$$\int \frac{(m + nx) dx}{\sqrt{a + bx}} = \frac{2}{3b^2} (3mb - 2an + nbx) \sqrt{a + bx} + C$$
33. 
$$\int \frac{dx}{(m + nx) \sqrt{a + bx}}$$
; substitute  $y = \sqrt{a + bx}$ , and use 21 and 22
34. 
$$\int \frac{f(x, \sqrt[n]{a + bx})}{F(x, \sqrt[n]{a + bx})} dx$$
; substitute  $\sqrt[n]{a + bx} = y$
35. 
$$\int \frac{dx}{\sqrt{a^2 - x^2}} = \sin^{-1} \frac{x}{a} + C = -\cos^{-1} \frac{x}{a} + C$$
36. 
$$\int \frac{dx}{\sqrt{a^2 + x^2}} = \ln(x + \sqrt{a^2 + x^2}) + C = \sinh^{-1} \frac{x}{a} + C$$
37. 
$$\int \frac{dx}{\sqrt{x^2 - a^2}} = \ln(x + \sqrt{x^2 - a^2}) + C = \cosh^{-1} \frac{x}{a} + C$$

**TABLE 2.24** Integrals (*Continued*)Irrational functions (*continued*)

38.  $\int \frac{dx}{\sqrt{a+2bx+cx^2}} = \frac{1}{\sqrt{c}} \ln(b+cx+\sqrt{c}\sqrt{a+2bx+cx^2}) + C$ , when  $c > 0$   
 $= \frac{1}{\sqrt{c}} \sinh^{-1} \frac{b+cx}{\sqrt{ac-b^2}} + C$ , when  $ac-b^2 > 0$   
 $= \frac{1}{\sqrt{c}} \cosh^{-1} \frac{b+cx}{\sqrt{b^2-ac}} + C$ , when  $b^2-ac > 0$   
 $= \frac{-1}{\sqrt{-c}} \sin^{-1} \frac{b+cx}{\sqrt{b^2-ac}} + C$ , when  $c < 0$
39.  $\int \frac{(m+nx) dx}{\sqrt{a+2bx+cx^2}} = \frac{n}{c} \sqrt{a+2bx+cx^2} + \frac{mc-nb}{c} \int \frac{dx}{\sqrt{a+2bx+cx^2}}$
40.  $\int \frac{x^m dx}{\sqrt{a+2bx+cx^2}} = \frac{x^{m-1} X}{mc} - \frac{(m-1)a}{mc} \int \frac{x^{m-2} dx}{X} - \frac{(2m-1)b}{mc} \int \frac{x^{m-1} dx}{X}$ ,  
 when  $X = \sqrt{a+2bx+cx^2}$
41.  $\int \sqrt{a^2+x^2} dx = \frac{x}{2} \sqrt{a^2+x^2} + \frac{a^2}{2} \ln(x+\sqrt{a^2+x^2}) + C$   
 $= \frac{x}{2} \sqrt{a^2+x^2} + \frac{a^2}{2} \sinh^{-1} \frac{x}{a} + C$
42.  $\int \sqrt{a^2-x^2} dx = \frac{x}{2} \sqrt{a^2-x^2} + \frac{a^2}{2} \sin^{-1} \frac{x}{a} + C$
43.  $\int \sqrt{x^2-a^2} dx = \frac{x}{2} \sqrt{x^2-a^2} - \frac{a^2}{2} \ln(x+\sqrt{x^2-a^2}) + C$   
 $= \frac{x}{2} \sqrt{x^2-a^2} - \frac{a^2}{2} \cosh^{-1} \frac{x}{a} + C$
44.  $\int \sqrt{a+2bx+cx^2} dx = \frac{b+cx}{2c} \sqrt{a+2bx+cx^2}$   
 $+ \frac{ac-b^2}{2c} \int \frac{dx}{\sqrt{a+2bx+cx^2}} + C$

## Transcendental functions

45.  $\int a^x dx = \frac{a^x}{\ln a} + C$
46.  $\int x^n e^{ax} dx = \frac{x^n e^{ax}}{a} \left[ 1 - \frac{n}{ax} + \frac{n(n-1)}{a^2 x^2} - \cdots \pm \frac{n!}{a^n x^n} \right] + C$
47.  $\int \ln x dx = x \ln x - x + C$
48.  $\int \frac{\ln x}{x^2} dx = -\frac{\ln x}{x} - \frac{1}{x} + C$
49.  $\int \frac{(\ln x)^n}{x} dx = \frac{1}{n+1} (\ln x)^{n+1} + C$
50.  $\int \sin^2 x dx = -\frac{1}{4} \sin 2x + \frac{1}{2} x + C = -\frac{1}{2} \sin x \cos x + \frac{1}{2} x + C$
51.  $\int \cos^2 x dx = \frac{1}{4} \sin 2x + \frac{1}{2} x + C = \frac{1}{2} \sin x \cos x + \frac{1}{2} x + C$
52.  $\int \sin mx dx = -\frac{\cos mx}{m} + C$
53.  $\int \cos mx dx = \frac{\sin mx}{m} + C$

**TABLE 2.24** Integrals (*Continued*)Transcendental functions (*continued*)

- 
54.  $\int \sin mx \cos nx \, dx = -\frac{\cos(m+n)x}{2(m+n)} - \frac{\cos(m-n)x}{2(m-n)} + C$
55.  $\int \sin mx \sin nx \, dx = \frac{\sin(m-n)x}{2(m-n)} - \frac{\sin(m+n)x}{2(m+n)} + C$
56.  $\int \cos mx \cos nx \, dx = \frac{\sin(m-n)x}{2(m-n)} + \frac{\sin(m+n)x}{2(m+n)} + C$
57.  $\int \tan x \, dx = -\ln \cos x + C$
58.  $\int \cot x \, dx = \ln \sin x + C$
59.  $\int \frac{dx}{\sin x} = \ln \tan \frac{x}{2} + C$
60.  $\int \frac{dx}{\cos x} = \ln \tan \left( \frac{\pi}{4} + \frac{x}{2} \right) + C$
61.  $\int \frac{dx}{1 + \cos x} = \tan \frac{x}{2} + C$
62.  $\int \frac{dx}{1 - \cos x} = -\cot \frac{x}{2} + C$
63.  $\int \sin x \cos x \, dx = \frac{1}{2} \sin^2 x + C$
64.  $\int \frac{dx}{\sin x \cos x} = \ln \tan x + C$
- 65.\*  $\int \sin^n x \, dx = -\frac{\cos x \sin^{n-1} x}{n} + \frac{n-1}{n} \int \sin^{n-2} x \, dx$
- 66.\*  $\int \cos^n x \, dx = \frac{\sin x \cos^{n-1} x}{n} + \frac{n-1}{n} \int \cos^{n-2} x \, dx$
67.  $\int \tan^n x \, dx = \frac{\tan^{n-1} x}{n-1} - \int \tan^{n-2} x \, dx$
68.  $\int \cot^n x \, dx = -\frac{\cot^{n-1} x}{n-1} - \int \cot^{n-2} x \, dx$
69.  $\int \frac{dx}{\sin^n x} = -\frac{\cos x}{(n-1) \sin^{n-1} x} + \frac{n-2}{n-1} \int \frac{dx}{\sin^{n-2} x}$
70.  $\int \frac{dx}{\cos^n x} = \frac{\sin x}{(n-1) \cos^{n-1} x} + \frac{n-2}{n-1} \int \frac{dx}{\cos^{n-2} x}$
- 71.\*  $\int \sin^p x \cos^q x \, dx = \frac{\sin^{p+1} x \cos^{q-1} x}{p+q} + \frac{q-1}{p+q} \int \sin^p x \cos^{q-2} x \, dx$   
 $= -\frac{\sin^{p-1} x \cos^{q+1} x}{p+q} + \frac{p-1}{p+q} \int \sin^{p-2} x \cos^q x \, dx$
- 72.\*  $\int \sin^{-p} x \cos^q x \, dx = -\frac{\sin^{-p+1} x \cos^{q+1} x}{p-1} + \frac{p-q-2}{p-1} \int \sin^{-p+2} x \cos^q x \, dx$
- 73.\*  $\int \sin^p x \cos^{-q} x \, dx = \frac{\sin^{p+1} x \cos^{-q+1} x}{q-1} + \frac{q-p-2}{q-1} \int \sin^p x \cos^{-q+2} x \, dx$
74.  $\int \frac{dx}{a + b \cos x} = \frac{2}{\sqrt{a^2 - b^2}} \tan^{-1} \left( \sqrt{\frac{a-b}{a+b}} \tan \frac{1}{2}x \right) + C, \text{ when } a^2 > b^2$   
 $= \frac{1}{\sqrt{b^2 - a^2}} \ln \frac{b + a \cos x + \sin x \sqrt{b^2 - a^2}}{a + b \cos x} + C$   
 $= \frac{2}{\sqrt{b^2 - a^2}} \tanh^{-1} \left( \sqrt{\frac{b-a}{b+a}} \tan \frac{1}{2}x \right) + C \quad \left. \vphantom{\int \frac{dx}{a + b \cos x}} \right\} [a^2 < b^2]$
75.  $\int \frac{\cos x \, dx}{a + b \cos x} = \frac{x}{b} - \frac{a}{b} \int \frac{dx}{a + b \cos x} + C$
- 

\* If  $n$ ,  $p$ , or  $q$  is an odd number, substitute  $\cos x = z$  or  $\sin x = z$

TABLE 2.24 Integrals (Continued)

| Transcendental functions (continued) |                                                                                                                                                                                                                                                                                                                                   |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 76.                                  | $\int \frac{\sin x \, dx}{a + b \cos x} = -\frac{1}{b} \ln (a + b \cos x) + C$                                                                                                                                                                                                                                                    |
| 77.                                  | $\int \frac{A + B \cos x + C \sin x}{a + b \cos x + c \sin x} dx = A \int \frac{dy}{a + p \cos y}$ $+ (B \cos u + C \sin u) \int \frac{\cos y \, dy}{a + p \cos y} - (B \sin u - C \cos u) \int \frac{\sin y \, dy}{a + p \cos y},$ <p>where <math>b = p \cos u</math>, <math>c = p \sin u</math>, and <math>x - u = y</math></p> |
| 78.                                  | $\int e^{ax} \sin bx \, dx = \frac{a \sin bx - b \cos bx}{a^2 + b^2} e^{ax} + C$                                                                                                                                                                                                                                                  |
| 79.                                  | $\int e^{ax} \cos bx \, dx = \frac{a \cos bx + b \sin bx}{a^2 + b^2} e^{ax} + C$                                                                                                                                                                                                                                                  |
| 80.                                  | $\int \sin^{-1} x \, dx = x \sin^{-1} x + \sqrt{1 - x^2} + C$                                                                                                                                                                                                                                                                     |
| 81.                                  | $\int \cos^{-1} x \, dx = x \cos^{-1} x - \sqrt{1 - x^2} + C$                                                                                                                                                                                                                                                                     |
| 82.                                  | $\int \tan^{-1} x \, dx = x \tan^{-1} x - \frac{1}{2} \ln(1 + x^2) + C$                                                                                                                                                                                                                                                           |
| 83.                                  | $\int \cot^{-1} x \, dx = x \cot^{-1} x + \frac{1}{2} \ln(1 + x^2) + C$                                                                                                                                                                                                                                                           |
| 84.                                  | $\int \sinh x \, dx = \cosh x + C$                                                                                                                                                                                                                                                                                                |
| 85.                                  | $\int \tanh x \, dx = \ln \cosh x + C$                                                                                                                                                                                                                                                                                            |
| 86.                                  | $\int \cosh x \, dx = \sinh x + C$                                                                                                                                                                                                                                                                                                |
| 87.                                  | $\int \coth x \, dx = \ln \sinh x + C$                                                                                                                                                                                                                                                                                            |
| 88.                                  | $\int \operatorname{sech} x \, dx = 2 \tan^{-1} (e^x) + C$                                                                                                                                                                                                                                                                        |
| 89.                                  | $\int \operatorname{csch} x \, dx = \ln \tanh \left( \frac{x}{2} \right) + C$                                                                                                                                                                                                                                                     |
| 90.                                  | $\int \sinh^2 x \, dx = \frac{1}{2} \sinh x \cosh x - \frac{1}{2} x + C$                                                                                                                                                                                                                                                          |
| 91.                                  | $\int \cosh^2 x \, dx = \frac{1}{2} \sinh x \cosh x + \frac{1}{2} x + C$                                                                                                                                                                                                                                                          |
| 92.                                  | $\int \operatorname{sech}^2 x \, dx = \tanh x + C$                                                                                                                                                                                                                                                                                |
| 93.                                  | $\int \operatorname{csch}^2 x \, dx = -\coth x + C$                                                                                                                                                                                                                                                                               |

2.2.2 Surface Areas and Volumes\*

Let  $a$ ,  $b$ ,  $c$ ,  $d$ , and  $s$  denote lengths,  $A$  denote areas, and  $V$  denote volumes.

*Triangle.*  $A = bh/2$ , where  $b$  denotes the base and  $h$  the altitude.

*Rectangle.*  $A = ab$ , where  $a$  and  $b$  denote the lengths of the sides.

*Parallelogram* (opposite sides parallel).  $A = ah = ab \sin \theta$ , where  $a$  and  $b$  denote the sides,  $h$  the altitude, and  $\theta$  the angle between the sides.

*Trapezoid* (four sides, two parallel).  $A = \frac{1}{2}h(a + b)$ , where  $a$  and  $b$  are the sides and  $h$  the altitude.

\* Adapted by permission from Burington, *Handbook of Mathematical Tables and Formulas*, 3d. ed., McGraw-Hill Book Company, New York (1959).

Regular Polygon of  $n$  Sides (Fig. 2.1)

$$A = \frac{1}{4} na^2 \cot \frac{180^\circ}{n} \quad \text{where } a \text{ is length of side}$$

$$R = \frac{a}{2} \csc \frac{180^\circ}{n} \quad \text{where } R \text{ is radius of circumscribed circle}$$

$$r = \frac{a}{2} \cot \frac{180^\circ}{n} \quad \text{where } r \text{ is radius of inscribed circle}$$

$$\alpha = \frac{360^\circ}{n} = \frac{2\pi}{n} \text{ radians}$$

$$\beta = \left( \frac{n-2}{n} \right) \cdot 180^\circ = \left( \frac{n-2}{n} \right) \pi \text{ radians} \quad \text{where } \alpha \text{ and } \beta \text{ are the angles indicated in Fig. 2.1}$$

$$a = 2r \tan \frac{\alpha}{2} = 2R \sin \frac{\alpha}{2}$$

Circle (Fig. 2.2). Let

$C$  = circumference       $S$  = length of arc subtended by  $\theta$

$R$  = radius       $l$  = chord subtended by arc  $S$

$D$  = diameter       $h$  = rise

$A$  = area       $\theta$  = central angle in radians

$$C = 2\pi R = \pi D \quad \pi = 3.14159 \dots$$

$$S = R\theta = \frac{1}{2}D\theta = D \cos^{-1} \frac{d}{R}$$

$$l = 2\sqrt{R^2 - d^2} = 2R \sin \frac{\theta}{2} = 2d \tan \frac{\theta}{2}$$

$$d = \frac{1}{2}\sqrt{4R^2 - l^2} = R \cos \frac{\theta}{2} = \frac{1}{2}l \cot \frac{\theta}{2}$$

$$h = R - d$$

$$\theta = \frac{S}{R} = \frac{2S}{D} = 2 \cos^{-1} \frac{d}{R} = 2 \tan^{-1} \frac{l}{2d} = 2 \sin^{-1} \frac{l}{D}$$

$$A (\text{circle}) = \pi R^2 = \frac{1}{4}\pi D^2$$

$$A (\text{sector}) = \frac{1}{2}Rs = \frac{1}{2}R^2\theta$$

$$A (\text{segment}) = A (\text{sector}) - A (\text{triangle}) = \frac{1}{2}R^2 (\theta - \sin \theta)$$

$$= R^2 \cos^{-1} \frac{R-h}{R} - (R-h)\sqrt{2Rh-h^2}$$

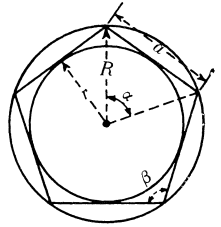


FIGURE 2.1

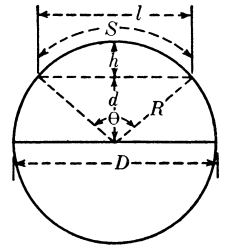


FIGURE 2.2

Perimeter of  $n$ -sided regular polygon inscribed in a circle  $= 2nR \sin \frac{\pi}{n}$

$$\text{Area of inscribed polygon} = \frac{1}{2}nR^2 \sin \frac{2\pi}{n}$$

Perimeter of  $n$ -sided regular polygon circumscribed about a circle  $= 2nR \tan \frac{\pi}{n}$

$$\text{Area of circumscribed polygon} = nR^2 \tan \frac{\pi}{n}$$

Radius of circle inscribed in a triangle of sides  $a$ ,  $b$ , and  $c$  is

$$r = \sqrt{\frac{(s-a)(s-b)(s-c)}{s}} \quad s = \frac{1}{2}(a+b+c)$$

Radius of circle circumscribed about a triangle is

$$R = \frac{abc}{4\sqrt{s(s-a)(s-b)(s-c)}}$$

*Ellipse* (Fig. 2.3).  $A = \pi ab$ , where  $a$  and  $b$  are lengths of semimajor and semiminor axes, respectively.

*Parabola* (Fig. 2.4)

$$A = \frac{2ld}{3}$$

$$\text{Height of } d_1 = \frac{d}{l^2} (l^2 - l_1^2)$$

$$\text{Width of } l_1 = l \sqrt{\frac{d-d_1}{d}}$$

$$\text{Length of arc} = l \left[ 1 + \frac{2}{3} \left( \frac{2d}{l} \right)^2 - \frac{2}{5} \left( \frac{2d}{l} \right)^4 + \cdots \right]$$

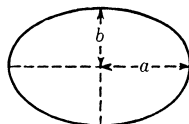


FIGURE 2.3

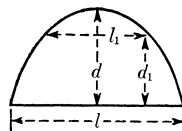


FIGURE 2.4

*Area by Approximation* (Fig. 2.5). If  $y_0, y_1, y_2, \dots, y_n$  are the length of a series of equally spaced parallel chords, and if  $h$  is their distance apart, the area enclosed by the boundary is given approximately by any one of the following formulae:

$$A_T = h[\frac{1}{2}(y_0 + y_n) + y_1 + y_2 + \cdots + y_{n-1}] \quad (\text{Trapezoidal Rule})$$

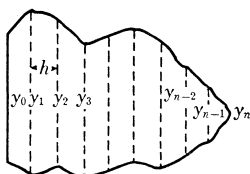


FIGURE 2.5

$A_D = h[0.4(y_0 + y_n) + 1.1(y_1 + y_{n-1}) + y_2 + y_3 + \cdots + y_{n-2}]$  (Durand's Rule)

$A_S = \frac{1}{3}h[(y_0 + y_n) + 4(y_1 + y_3 + \cdots + y_{n-1}) + 2(y_2 + y_4 + \cdots + y_{n-2})]$   
( $n$  even, Simpson's Rule)

In general,  $A_S$  gives the most accurate approximation.  
The greater the value of  $n$ , the greater the accuracy of approximation.

*Cube.*  $V = a^3$ ;  $d = a\sqrt{2}$ ; total surface area =  $6a^2$ , where  $a$  is length of side and  $d$  is length of diagonal.

*Rectangular Parallelopiped.*  $V = abc$ ;  $d = \sqrt{a^2 + b^2 + c^2}$ ; total surface area =  $2(ab + bc + ca)$ , where  $a$ ,  $b$ , and  $c$  are the lengths of the sides and  $d$  is length of diagonal.

*Prism or Cylinder*

$V = (\text{area of base}) \cdot (\text{altitude})$

Lateral area = (perimeter of right section)  $\cdot$  (lateral edge)

*Pyramid or Cone*

$V = \frac{1}{3}(\text{area of base}) \cdot (\text{altitude})$

Lateral area of regular pyramid =  $\frac{1}{2}(\text{perimeter of base}) \cdot (\text{slant height})$

*Frustum of Pyramid or Cone.*  $V = \frac{1}{3}(A_1 + A_2 + \sqrt{A_1 \cdot A_2})h$ , where  $h$  is the altitude and  $A_1$  and  $A_2$  are the areas of the bases.

Lateral area of a regular figure =  $\frac{1}{2}(\text{sum of perimeters of base}) \cdot (\text{slant height})$

*Prismoid*

$V = \frac{h}{6} (A_1 + A_2 + 4A_3)$

where  $h$  = altitude,  $A_1$  and  $A_2$  are the areas of the bases, and  $A_3$  is the area of the midsection parallel to bases.

*Area of Surface and Volume of Regular Polyhedra of Edge  $l$*

| Name              | Type of surface          | Area of surface | Volume       |
|-------------------|--------------------------|-----------------|--------------|
| Tetrahedron       | 4 equilateral triangles  | $1.73205l^2$    | $0.11785l^3$ |
| Hexahedron (cube) | 6 squares                | $6.00000l^2$    | $1.00000l^3$ |
| Octahedron        | 8 equilateral triangles  | $3.46410l^2$    | $0.47140l^3$ |
| Dodecahedron      | 12 pentagons             | $20.64578l^2$   | $7.66312l^3$ |
| Icosahedron       | 20 equilateral triangles | $8.66025l^2$    | $2.18170l^3$ |

*Sphere (Fig. 2.6)*

$A \text{ (sphere)} = 4\pi R^2 = \pi D^2$

$A \text{ (zone)} = 2\pi Rh_1 = \pi Dh_1$

$V \text{ (sphere)} = \frac{4}{3}\pi R^3 = \frac{1}{8}\pi D^3$



$$V (\text{spherical sector}) = \frac{2}{3}\pi R^2 h_1 = \frac{1}{6}\pi D^2 h_1$$

$$V (\text{spherical segment of one base}) = \frac{1}{6}\pi h_3 (3r_3^2 + h_3^2)$$

$$V (\text{spherical segment of two bases}) = \frac{1}{6}\pi h_2 (3r_3^2 + 3r_2^2 + h_2^2)$$

$$A (\text{lune}) = 2R^2 \theta \quad \text{where } \theta \text{ is angle in radians of lune}$$

*Ellipsoid.*  $V = \frac{4}{3}\pi abc$ , where  $a$ ,  $b$ , and  $c$  are the lengths of the semiaxes.

*Torus* (Fig. 2.7)

$$V = 2\pi^2 R r^2$$

$$\text{Area of surface} = S = 4\pi^2 R r$$

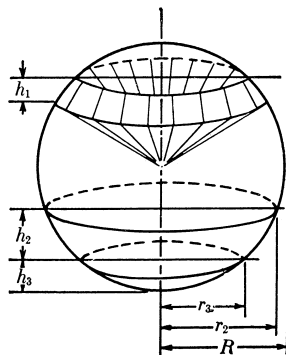


FIGURE 2.6

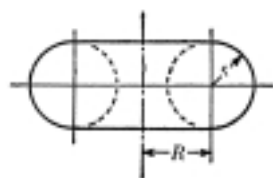


FIGURE 2.7

## 2.2.3 Trigonometric Functions of an Angle $\alpha$

Let  $x$  be any angle whose initial side lies on the positive  $x$  axis and whose vertex is at the origin, and  $(x, y)$  be any point on the terminal side of the angle. ( $x$  is positive if measured along  $OX$  to the right, from the  $y$  axis; and negative, if measured along  $OX'$  to the left from the  $y$  axis. Likewise,  $y$  is positive if measured parallel to  $OY$ , and negative if measured parallel to  $OY'$ .) Let  $r$  be the positive distance from the origin to the point. The trigonometric functions of an angle are defined as follows:

$$\text{sine } \alpha = \sin \alpha = \frac{y}{r}$$

$$\text{cosine } \alpha = \cos \alpha = \frac{x}{r}$$

$$\text{tangent } \alpha = \tan \alpha = \frac{y}{x}$$

$$\text{cotangent } \alpha = \text{ctn } \alpha = \cot \alpha = \frac{x}{y}$$

$$\text{secant } \alpha = \sec \alpha = \frac{r}{x}$$

$$\text{cosecant } \alpha = \csc \alpha = \frac{r}{y}$$

$$\text{exsecant } \alpha = \text{exsec } \alpha = \sec \alpha - 1$$

$$\text{versine } \alpha = \text{vers } \alpha = 1 - \cos \alpha$$

$$\text{coversine } \alpha = \text{covers } \alpha = 1 - \sin \alpha$$

$$\text{haversine } \alpha = \text{hav } \alpha = \frac{1}{2} \text{vers } \alpha$$

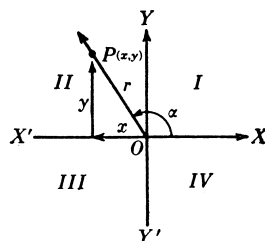


FIGURE 2.8

### 2.2.3.1 Signs of the Functions

| Quadrant | sin | cos | tan | ctn | sec | csc |
|----------|-----|-----|-----|-----|-----|-----|
| I        | +   | +   | +   | +   | +   | +   |
| II       | +   | -   | -   | -   | -   | +   |
| III      | -   | -   | +   | +   | -   | -   |
| IV       | -   | +   | -   | -   | +   | -   |

### 2.2.3.2 Relations between the Functions of a Single Angle\*

$$\sin^2 x + \cos^2 x = 1$$

$$\tan x = \frac{\sin x}{\cos x}$$

$$\cot x = \frac{1}{\tan x} = \frac{\cos x}{\sin x}$$

$$1 + \tan^2 x = \sec^2 x = \frac{1}{\cos^2 x}$$

$$1 + \cot^2 x = \csc^2 x = \frac{1}{\sin^2 x}$$

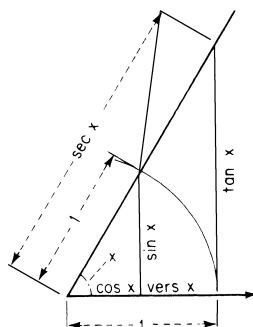


FIGURE 2.9

$$\sin x = \sqrt{1 - \cos^2 x} = \frac{\tan x}{\sqrt{1 + \tan^2 x}} = \frac{1}{\sqrt{1 + \cot^2 x}}$$

$$\cos x = \sqrt{1 - \sin^2 x} = \frac{1}{\sqrt{1 + \tan^2 x}} = \frac{\cot x}{\sqrt{1 + \cot^2 x}}$$

**2.2.3.3 Functions of Negative Angles.**  $\sin(-x) = -\sin x$ ;  $\cos(-x) = \cos x$ ;  $\tan(-x) = -\tan x$ .

### 2.2.3.4 Functions of the Sum and Difference of Two Angles

$$\sin(x + y) = \sin x \cos y + \cos x \sin y$$

$$\cos(x + y) = \cos x \cos y - \sin x \sin y$$

$$\tan(x + y) = \frac{\tan x + \tan y}{1 - \tan x \tan y}$$

$$\cot(x + y) = \frac{\cot x \cot y - 1}{\cot x + \cot y}$$

$$\sin(x - y) = \sin x \cos y - \cos x \sin y$$

\* From Baumeister and Marks, *Standard Handbook for Mechanical Engineers*, 7th ed., McGraw-Hill Book Company, New York (1967); by permission.

$$\cos(x - y) = \cos x \cos y + \sin x \sin y$$

$$\tan(x - y) = \frac{\tan x - \tan y}{1 + \tan x \tan y}$$

$$\cot(x - y) = \frac{\cot x \cot y + 1}{\cot y - \cot x}$$

$$\sin x + \sin y = 2 \sin \frac{1}{2}(x + y) \cos \frac{1}{2}(x - y)$$

$$\sin x - \sin y = 2 \cos \frac{1}{2}(x + y) \sin \frac{1}{2}(x - y)$$

$$\cos x + \cos y = 2 \cos \frac{1}{2}(x + y) \cos \frac{1}{2}(x - y)$$

$$\cos x - \cos y = -2 \sin \frac{1}{2}(x + y) \sin \frac{1}{2}(x - y)$$

$$\tan x + \tan y = \frac{\sin(x + y)}{\cos x \cos y} \quad \cot x + \cot y = \frac{\sin(x + y)}{\sin x \sin y}$$

$$\tan x - \tan y = \frac{\sin(x - y)}{\cos x \cos y} \quad \cot x - \cot y = \frac{\sin(y - x)}{\sin x \sin y}$$

$$\sin^2 x - \sin^2 y = \cos^2 y - \cos^2 x = \sin(x + y) \sin(x - y)$$

$$\cos^2 x - \sin^2 y = \cos^2 y - \sin^2 x = \cos(x + y) \cos(x - y)$$

$$\sin(45^\circ + x) = \cos(45^\circ - x) \quad \tan(45^\circ + x) = \cot(45^\circ - x)$$

$$\sin(45^\circ - x) = \cos(45^\circ + x) \quad \tan(45^\circ - x) = \cot(45^\circ + x)$$

In the following transformations,  $a$  and  $b$  are supposed to be positive,  $c = \sqrt{a^2 + b^2}$ ,  $A =$  the positive acute angle for which  $B = b/a$ :

$$a \cos x + b \sin x = c \sin(A + x) = c \cos(B - x)$$

$$a \cos x - b \sin x = c \sin(A - x) = c \cos(B + x)$$

## 2.2.4 Expansion in Series\*

The range of values of  $x$  for which each of the series is convergent is stated at the right of the series.

### 2.2.4.1 Exponential and Logarithmic Series

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots \quad (-\infty < x < +\infty)$$

$$a^x = e^{mx} = 1 + \frac{m}{1!}x + \frac{m^2}{2!}x^2 + \frac{m^3}{3!}x^3 + \cdots \quad (a > 0, -\infty < x < +\infty)$$

where  $m = \ln a = 2.3026 \log_{10} a$ .

\* From Baumeister and Marks, *Standard Handbook for Mechanical Engineers*, 7th ed., McGraw-Hill Book Company, New York (1967); by permission.

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \frac{x^5}{5} \cdots \quad (-1 < x < +1)$$

$$\ln(1-x) = -x - \frac{x^2}{2} - \frac{x^3}{3} - \frac{x^4}{4} - \frac{x^5}{5} - \cdots \quad (-1 < x < +1)$$

$$\ln\left(\frac{1+x}{1-x}\right) = 2\left(x + \frac{x^3}{3} + \frac{x^5}{5} + \frac{x^7}{7} + \cdots\right) \quad (-1 < x < +1)$$

$$\ln\left(\frac{x+1}{x-1}\right) = 2\left(\frac{1}{x} + \frac{1}{3x^3} + \frac{1}{5x^5} + \frac{1}{7x^7} + \cdots\right) \quad (x < -1 \text{ or } +1 < x)$$

$$\ln x = 2\left[\frac{x-1}{x+1} + \frac{1}{3}\left(\frac{x-1}{x+1}\right)^3 + \frac{1}{5}\left(\frac{x-1}{x+1}\right)^5 + \cdots\right] \quad (0 < x < \infty)$$

$$\ln(a+x) = \ln a + 2\left[\frac{x}{2a+x} + \frac{1}{3}\left(\frac{x}{2a+x}\right)^3 + \frac{1}{5}\left(\frac{x}{2a+x}\right)^5 + \cdots\right] \\ (0 < a < +\infty, -a < x < +\infty)$$

*Series for the Trigonometric Functions.* In the following formulas, *all angles must be expressed in radians*. If  $D$  = the number of degrees in the angle, and  $x$  = its radian measure, then  $x = 0.017453D$ .

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \quad (-\infty < x < +\infty)$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} - \cdots \quad (-\infty < x < +\infty)$$

$$\tan x = x + \frac{x^3}{3} + \frac{2x^5}{15} + \frac{17x^7}{315} + \frac{62x^9}{2835} + \cdots \quad \left(-\frac{\pi}{2} < x < +\frac{\pi}{2}\right)$$

$$\cot x = \frac{1}{x} - \frac{x}{3} - \frac{x^3}{45} - \frac{2x^5}{945} - \frac{x^7}{4725} - \cdots \quad (-\pi < x < +\pi)$$

$$\sin^{-1} y = y + \frac{y^3}{6} + \frac{3y^5}{40} + \frac{5y^7}{112} + \cdots \quad (-1 \leq y \leq +1)$$

$$\tan^{-1} y = y - \frac{y^3}{3} + \frac{y^5}{5} - \frac{y^7}{7} + \cdots \quad (-1 \leq y \leq +1)$$

$$\cos^{-1} y = \frac{1}{2}\pi - \sin^{-1} y \quad \cot^{-1} y = \frac{1}{2}\pi - \tan^{-1} y$$

*Reversing a Series.* If  $y = x + bx^2 + cx^3 + dx^4 + ex^5 + \cdots$ , then  $x = y - by^2 + (2b^2 - c)y^3 - (5b^3 - 5bc + d)y^4 + (14b^4 - 21b^2c + 6bd + 3c^2 - e)y^5 + \cdots$ , provided the latter series is convergent.

*Fourier's Series.* Let  $f(x)$  be a function which is finite in the interval from  $x = -c$  to  $x = +c$  and whose graph has finite arc length in that interval.\* Then, for any value of  $x$  between  $-c$  and  $c$ ,

\* If  $x = x_0$  is a point of discontinuity,  $f(x_0)$  is to be defined as  $\frac{1}{2}[f_1(x_0) + f_2(x_0)]$ , where  $f_1(x_0)$  is the limit of  $f(x)$  when  $x$  approaches  $x_0$  from below, and  $f_2(x_0)$  is the limit of  $f(x)$  when  $x$  approaches  $x_0$  from above.

$$f(x) = \frac{1}{2}a_0 + a_1 \cos \frac{\pi x}{c} + a_2 \cos \frac{2\pi x}{c} + a_3 \cos \frac{3\pi x}{c} + \cdots$$

$$+ b_1 \sin \frac{\pi x}{c} + b_2 \sin \frac{2\pi x}{c} + b_3 \sin \frac{3\pi x}{c} + \cdots$$

where the constant coefficients are determined as follows:

$$a_n = \frac{1}{c} \int_{-c}^c f(t) \cos \frac{n\pi t}{c} dt$$

$$b_n = \frac{1}{c} \int_{-c}^c f(t) \sin \frac{n\pi t}{c} dt$$

In case the curve  $y = f(x)$  is symmetrical with respect to the origin, the  $a$ 's are all zero, and the series is a sine series. In case the curve is symmetrical with respect to the  $y$  axis, the  $b$ 's are all zero, and a cosine series results. (In this case, the series will be valid not only for values of  $x$  between  $-c$  and  $c$ , but also for  $x = -c$  and  $x = c$ .) A Fourier series can always be integrated term by term; but the result of differentiating term by term may not be a convergent series.

TABLE 2.25 Some Constants

| Constant                                    | Number                    | Log <sub>10</sub> of Number    |
|---------------------------------------------|---------------------------|--------------------------------|
| Pi ( $\pi$ )                                | 3.14159 26535 89793 23846 | 0.49714 98726 94133 85435      |
| Napierian Base ( $e$ )                      | 2.71828 18284 59045 23536 | 0.43429 448                    |
| $M = \log_{10}e$                            | 0.43429 44819 03251 82765 | 9.63778 43113 00536 78912 - 10 |
| $1 \div M = \log_e 10$                      | 2.30258 50929 94045 68402 | 0.36221 569                    |
| $180 \div \pi = \text{degrees in 1 radian}$ | 57.2957 795               | 1.75812 263                    |
| $\pi \div 180 = \text{radians in } 1^\circ$ | 0.01745 329               | 8.24187 737 - 10               |
| $\pi \div 10800 = \text{radians in } 1'$    | 0.00029 08882             | 6.46372 612 - 10               |
| $\pi \div 648000 = \text{radians in } 1''$  | 0.00000 48481 36811 095   | 4.68557 487 - 10               |

2.3 STATISTICS IN CHEMICAL ANALYSIS

2.3.1 Introduction

Each observation in any branch of scientific investigation is inaccurate to some degree. Often the accurate value for the concentration of some particular constituent in the analyte cannot be determined. However, it is reasonable to assume the accurate value exists, and it is important to estimate the limits between which this value lies. It must be understood that the statistical approach is concerned with the appraisal of experimental design and data. Statistical techniques can neither detect nor evaluate constant errors (bias); the detection and elimination of inaccuracy are analytical problems. Nevertheless, statistical techniques can assist considerably in determining whether or not inaccuracies exist and in indicating when procedural modifications have reduced them.

By proper design of experiments, guided by a statistical approach, the effects of experimental variables may be found more efficiently than by the traditional approach of holding all variables constant but one and systematically investigating each variable in turn. Trends in data may be sought to track down nonrandom sources of error.

### 2.3.2 Errors in Quantitative Analysis

Two broad classes of errors may be recognized. The first class, *determinate* or *systematic* errors, is composed of errors that can be assigned to definite causes, even though the cause may not have been located. Such errors are characterized by being unidirectional. The magnitude may be constant from sample to sample, proportional to sample size, or variable in a more complex way. An example is the error caused by weighing a hygroscopic sample. This error is always positive in sign; it increases with sample size but varies depending on the time required for weighing, with humidity and temperature. An example of a negative systematic error is that caused by solubility losses of a precipitate.

The second class, *indeterminate* or *random* errors, is brought about by the effects of uncontrolled variables. Truly random errors are as likely to cause high as low results, and a small random error is much more probable than a large one. By making the observation coarse enough, random errors would cease to exist. Every observation would give the same result, but the result would be less precise than the average of a number of finer observations with random scatter.

The *precision* of a result is its reproducibility; the *accuracy* is its nearness to the truth. A systematic error causes a loss of accuracy, and it may or may not impair the precision depending upon whether the error is constant or variable. Random errors cause a lowering of reproducibility, but by making sufficient observations it is possible to overcome the scatter within limits so that the accuracy may not necessarily be affected. Statistical treatment can properly be applied only to random errors.

### 2.3.3 Representation of Sets of Data

Raw data are collected observations that have not been organized numerically. An *average* is a value that is typical or representative of a set of data. Several averages can be defined, the most common being the arithmetic mean (or briefly, the mean), the median, the mode, and the geometric mean.

The *mean* of a set of  $N$  numbers,  $x_1, x_2, x_3, \dots, x_N$ , is denoted by  $\bar{x}$  and is defined as:

$$\bar{x} = \frac{x_1 + x_2 + x_3 + \dots + x_N}{N} \quad (2.4)$$

It is an estimation of the unknown true value  $\mu$  of an infinite population. We can also define the *sample variance*  $s^2$  as follows:

$$s^2 = \frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N - 1} \quad (2.5)$$

The values of  $\bar{x}$  and  $s^2$  vary from sample set to sample set. However, as  $N$  increases, they may be expected to become more and more stable. Their limiting values, for very large  $N$ , are numbers characteristic of the frequency distribution, and are referred to as the *population mean* and the *population variance*, respectively.

The *median* of a set of numbers arranged in order of magnitude is the middle value or the arithmetic mean of the two middle values. The median allows inclusion of all data in a set without undue influence from outlying values; it is preferable to the mean for small sets of data.

The *mode* of a set of numbers is that value which occurs with the greatest frequency (the most common value). The mode may not exist, and even if it does exist it may not be unique. The empirical relation that exists between the mean, the mode, and the median for unimodal frequency curves which are moderately asymmetrical is:

$$\text{Mean} - \text{mode} = 3(\text{mean} - \text{median}) \quad (2.6)$$

The *geometric mean* of a set of  $N$  numbers is the  $N$ th root of the product of the numbers:

$$\sqrt[N]{x_1 x_2 x_3 \dots x_N} \quad (2.7)$$

The *root mean square* (RMS) or quadratic mean of a set of numbers is defined by:

$$\text{RMS} = \sqrt{\bar{x}^2} = \sqrt{\sum_{i=1}^N x_i^2 / N} \quad (2.8)$$

### 2.3.4 The Normal Distribution of Measurements

The normal distribution of measurements (or the normal law of error) is the fundamental starting point for analysis of data. When a large number of measurements are made, the individual measurements are not all identical and equal to the accepted value  $\mu$ , which is the mean of an infinite population or universe of data, but are scattered about  $\mu$ , owing to random error. If the magnitude of any single measurement is the abscissa and the relative frequencies (i.e., the probability) of occurrence of different-sized measurements are the ordinate, the smooth curve drawn through the points (Fig. 2.10) is the *normal* or *Gaussian distribution curve* (also the *error curve* or *probability curve*). The term *error curve* arises when one considers the distribution of errors ( $x - \mu$ ) about the true value.

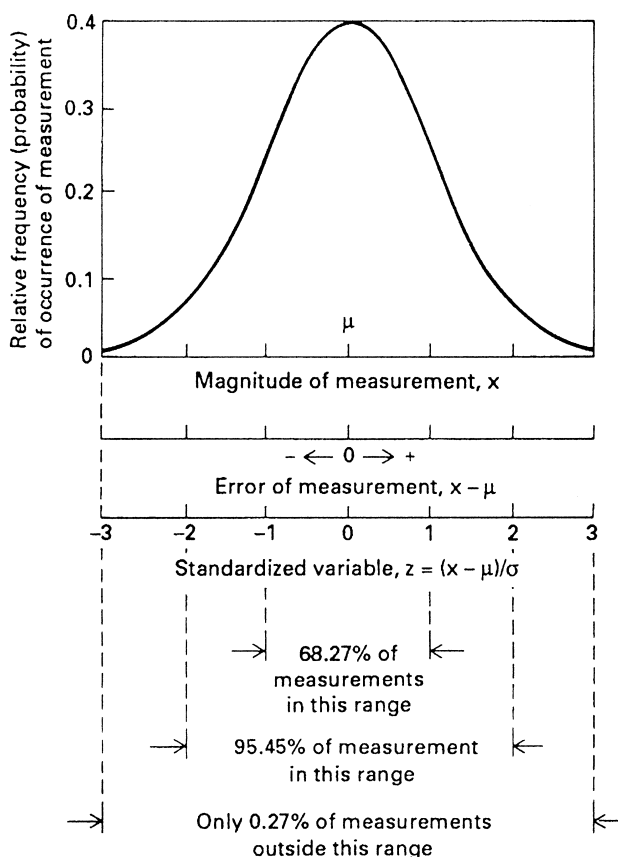


FIGURE 2.10 The Normal Distribution Curve.

The breadth or spread of the curve indicates the precision of the measurements and is determined by and related to the standard deviation, a relationship that is expressed in the equation for the normal curve (which is continuous and infinite in extent):

$$Y = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{x - \mu}{\sigma} \right)^2 \right] \quad (2.9)$$

where  $\sigma$  is the standard deviation of the infinite population. The population mean  $\mu$  expresses the magnitude of the quantity being measured. In a sense,  $\sigma$  measures the width of the distribution, and thereby also expresses the scatter or dispersion of replicate analytical results. When  $(x - \mu)/\sigma$  is replaced by the standardized variable  $z$ , then:

$$Y = \frac{1}{\sqrt{2\pi}} e^{-(1/2)z^2} \quad (2.10)$$

The standardized variable (the  $z$  statistic) requires only the probability level to be specified. It measures the deviation from the population mean in units of standard deviation.  $Y$  is 0.399 for the most probable value,  $\mu$ . In the absence of any other information, the normal distribution is assumed to apply whenever repetitive measurements are made on a sample, or a similar measurement is made on different samples.

Table 2.26a lists the height of an ordinate ( $Y$ ) as a distance  $z$  from the mean, and Table 2.26b the area under the normal curve at a distance  $z$  from the mean, expressed as fractions of the total area, 1.000. Returning to Fig. 2.10, we note that 68.27% of the area of the normal distribution curve lies within 1 standard deviation of the center or mean value. Therefore, 31.73% lies outside those limits and 15.86% on each side. Ninety-five percent (actually 95.43%) of the area lies within 2 standard deviations, and 99.73% lies within 3 standard deviations of the mean. Often the last two areas are stated slightly different; viz. 95% of the area lies within  $1.96\sigma$  (approximately  $2\sigma$ ) and 99% lies within approximately  $2.5\sigma$ . The mean falls at exactly the 50% point for symmetric normal distributions.

**Example 5** The true value of a quantity is 30.00, and  $\sigma$  for the method of measurement is 0.30. What is the probability that a single measurement will have a deviation from the mean greater than 0.45; that is, what percentage of results will fall outside the range  $30.00 \pm 0.45$ ?

$$z = \frac{x - \mu}{\sigma} = \frac{0.45}{0.30} = 1.5$$

From Table 2.26b the area under the normal curve from  $-1.5\sigma$  to  $+1.5\sigma$  is 0.866, meaning that 86.6% of the measurements will fall within the range  $30.00 \pm 0.45$  and 13.4% will lie outside this range. Half of these measurements, 6.7%, will be less than 29.55; and a similar percentage will exceed 30.45. In actuality the uncertainty in  $z$  is about 1 in 15; therefore, the value of  $z$  could lie between 1.4 and 1.6; the corresponding areas under the curve could lie between 84% and 89%.

**Example 6** If the mean value of 500 determinations is 151 and  $\sigma = 15$ , how many results lie between 120 and 155 (actually any value between 119.5 and 155.5)?

$$z = \frac{119.5 - 151}{15} = -2.10 \quad \text{Area: 0.482}$$

$$z = \frac{155.5 - 151}{15} = 0.30 \quad 0.118$$

Total area: 0.600

$$500(0.600) = 300 \text{ results}$$



**TABLE 2.26a** Ordinates (Y) of the Normal Distribution Curve at Values of z

| z   | 0      | 1      | 2      | 3      | 4      | 5      | 6      | 7      | 8      | 9      |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 0.0 | 0.3989 | 0.3989 | 0.3989 | 0.3988 | 0.3986 | 0.3984 | 0.3982 | 0.3980 | 0.3977 | 0.3973 |
| 0.1 | 0.3970 | 0.3965 | 0.3961 | 0.3956 | 0.3951 | 0.3945 | 0.3939 | 0.3932 | 0.3925 | 0.3918 |
| 0.2 | 0.3910 | 0.3902 | 0.3894 | 0.3885 | 0.3876 | 0.3867 | 0.3857 | 0.3847 | 0.3836 | 0.3825 |
| 0.3 | 0.3814 | 0.3802 | 0.3790 | 0.3778 | 0.3765 | 0.3752 | 0.3739 | 0.3725 | 0.3712 | 0.3697 |
| 0.4 | 0.3683 | 0.3668 | 0.3653 | 0.3637 | 0.3621 | 0.3605 | 0.3589 | 0.3572 | 0.3555 | 0.3538 |
| 0.5 | 0.3521 | 0.3503 | 0.3485 | 0.3467 | 0.3448 | 0.3429 | 0.3410 | 0.3391 | 0.3372 | 0.3352 |
| 0.6 | 0.3332 | 0.3312 | 0.3292 | 0.3271 | 0.3251 | 0.3230 | 0.3209 | 0.3187 | 0.3166 | 0.3144 |
| 0.7 | 0.3123 | 0.3101 | 0.3079 | 0.3056 | 0.3034 | 0.3011 | 0.2989 | 0.2966 | 0.2943 | 0.2920 |
| 0.8 | 0.2897 | 0.2874 | 0.2850 | 0.2827 | 0.2803 | 0.2780 | 0.2756 | 0.2732 | 0.2709 | 0.2685 |
| 0.9 | 0.2661 | 0.2637 | 0.2613 | 0.2589 | 0.2565 | 0.2541 | 0.2516 | 0.2492 | 0.2468 | 0.2444 |
| 1.0 | 0.2420 | 0.2396 | 0.2371 | 0.2347 | 0.2323 | 0.2299 | 0.2275 | 0.2251 | 0.2227 | 0.2203 |
| 1.1 | 0.2179 | 0.2155 | 0.2131 | 0.2107 | 0.2083 | 0.2059 | 0.2036 | 0.2012 | 0.1989 | 0.1965 |
| 1.2 | 0.1942 | 0.1919 | 0.1895 | 0.1872 | 0.1849 | 0.1826 | 0.1804 | 0.1781 | 0.1758 | 0.1736 |
| 1.3 | 0.1714 | 0.1691 | 0.1669 | 0.1647 | 0.1626 | 0.1604 | 0.1582 | 0.1561 | 0.1539 | 0.1518 |
| 1.4 | 0.1497 | 0.1476 | 0.1456 | 0.1435 | 0.1415 | 0.1394 | 0.1374 | 0.1354 | 0.1334 | 0.1315 |
| 1.5 | 0.1295 | 0.1276 | 0.1257 | 0.1238 | 0.1219 | 0.1200 | 0.1182 | 0.1163 | 0.1145 | 0.1127 |
| 1.6 | 0.1109 | 0.1092 | 0.1074 | 0.1057 | 0.1040 | 0.1023 | 0.1006 | 0.0989 | 0.0973 | 0.0957 |
| 1.7 | 0.0940 | 0.0925 | 0.0909 | 0.0893 | 0.0878 | 0.0863 | 0.0848 | 0.0833 | 0.0818 | 0.0804 |
| 1.8 | 0.0790 | 0.0775 | 0.0761 | 0.0748 | 0.0734 | 0.0721 | 0.0707 | 0.0694 | 0.0681 | 0.0669 |
| 1.9 | 0.0656 | 0.0644 | 0.0632 | 0.0620 | 0.0608 | 0.0596 | 0.0584 | 0.0573 | 0.0562 | 0.0551 |
| 2.0 | 0.0540 | 0.0529 | 0.0519 | 0.0508 | 0.0498 | 0.0488 | 0.0478 | 0.0468 | 0.0459 | 0.0449 |
| 2.1 | 0.0440 | 0.0431 | 0.0422 | 0.0413 | 0.0404 | 0.0396 | 0.0387 | 0.0379 | 0.0371 | 0.0363 |
| 2.2 | 0.0355 | 0.0347 | 0.0339 | 0.0332 | 0.0325 | 0.0317 | 0.0310 | 0.0303 | 0.0297 | 0.0290 |
| 2.3 | 0.0283 | 0.0277 | 0.0270 | 0.0264 | 0.0258 | 0.0252 | 0.0246 | 0.0241 | 0.0235 | 0.0229 |
| 2.4 | 0.0224 | 0.0219 | 0.0213 | 0.0208 | 0.0203 | 0.0198 | 0.0194 | 0.0189 | 0.0184 | 0.0180 |
| 2.5 | 0.0175 | 0.0171 | 0.0167 | 0.0163 | 0.0158 | 0.0154 | 0.0151 | 0.0147 | 0.0143 | 0.0139 |
| 2.6 | 0.0136 | 0.0132 | 0.0129 | 0.0126 | 0.0122 | 0.0119 | 0.0116 | 0.0113 | 0.0110 | 0.0107 |
| 2.7 | 0.0104 | 0.0101 | 0.0099 | 0.0096 | 0.0093 | 0.0091 | 0.0088 | 0.0086 | 0.0084 | 0.0081 |
| 2.8 | 0.0079 | 0.0077 | 0.0075 | 0.0073 | 0.0071 | 0.0069 | 0.0067 | 0.0065 | 0.0063 | 0.0061 |
| 2.9 | 0.0060 | 0.0058 | 0.0056 | 0.0055 | 0.0053 | 0.0051 | 0.0050 | 0.0048 | 0.0047 | 0.0046 |
| 3.0 | 0.0044 | 0.0043 | 0.0042 | 0.0040 | 0.0039 | 0.0038 | 0.0037 | 0.0036 | 0.0035 | 0.0034 |
| 3.1 | 0.0033 | 0.0032 | 0.0031 | 0.0030 | 0.0029 | 0.0028 | 0.0027 | 0.0026 | 0.0025 | 0.0025 |
| 3.2 | 0.0024 | 0.0023 | 0.0022 | 0.0022 | 0.0021 | 0.0020 | 0.0020 | 0.0019 | 0.0018 | 0.0018 |
| 3.3 | 0.0017 | 0.0017 | 0.0016 | 0.0016 | 0.0015 | 0.0015 | 0.0014 | 0.0014 | 0.0013 | 0.0013 |
| 3.4 | 0.0012 | 0.0012 | 0.0012 | 0.0011 | 0.0011 | 0.0010 | 0.0010 | 0.0010 | 0.0009 | 0.0009 |
| 3.5 | 0.0009 | 0.0008 | 0.0008 | 0.0008 | 0.0008 | 0.0007 | 0.0007 | 0.0007 | 0.0007 | 0.0006 |
| 3.6 | 0.0006 | 0.0006 | 0.0006 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0004 |
| 3.7 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0004 | 0.0003 | 0.0003 | 0.0003 | 0.0003 |
| 3.8 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 |
| 3.9 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0001 | 0.0001 |

2.3.5 Standard Deviation as a Measure of Dispersion

Several ways may be used to characterize the spread or dispersion in the original data. The *range* is the difference between the largest value and the smallest value in a set of observations. However, almost always the most efficient quantity for characterizing variability is the *standard deviation* (also called the *root mean square*).

**TABLE 2.26b** Areas Under the Normal Distribution Curve from 0 to z

| z   | 0      | 1      | 2      | 3      | 4      | 5      | 6      | 7      | 8      | 9      |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 0.0 | 0.0000 | 0.0040 | 0.0080 | 0.0120 | 0.0160 | 0.0199 | 0.0239 | 0.0279 | 0.0319 | 0.0359 |
| 0.1 | 0.0398 | 0.0438 | 0.0478 | 0.0517 | 0.0557 | 0.0596 | 0.0636 | 0.0675 | 0.0714 | 0.0754 |
| 0.2 | 0.0793 | 0.0832 | 0.0871 | 0.0910 | 0.0948 | 0.0987 | 0.1026 | 0.1064 | 0.1103 | 0.1141 |
| 0.3 | 0.1179 | 0.1217 | 0.1255 | 0.1293 | 0.1331 | 0.1368 | 0.1406 | 0.1443 | 0.1480 | 0.1517 |
| 0.4 | 0.1554 | 0.1591 | 0.1628 | 0.1664 | 0.1700 | 0.1736 | 0.1772 | 0.1808 | 0.1844 | 0.1879 |
| 0.5 | 0.1915 | 0.1950 | 0.1985 | 0.2019 | 0.2054 | 0.2088 | 0.2123 | 0.2157 | 0.2190 | 0.2224 |
| 0.6 | 0.2258 | 0.2291 | 0.2324 | 0.2357 | 0.2389 | 0.2422 | 0.2454 | 0.2486 | 0.2518 | 0.2549 |
| 0.7 | 0.2580 | 0.2612 | 0.2642 | 0.2673 | 0.2704 | 0.2734 | 0.2764 | 0.2794 | 0.2823 | 0.2852 |
| 0.8 | 0.2881 | 0.2910 | 0.2939 | 0.2967 | 0.2996 | 0.3023 | 0.3051 | 0.3078 | 0.3106 | 0.3133 |
| 0.9 | 0.3159 | 0.3186 | 0.3212 | 0.3238 | 0.3264 | 0.3289 | 0.3315 | 0.3340 | 0.3365 | 0.3389 |
| 1.0 | 0.3413 | 0.3438 | 0.3461 | 0.3485 | 0.3508 | 0.3531 | 0.3554 | 0.3577 | 0.3599 | 0.3621 |
| 1.1 | 0.3643 | 0.3665 | 0.3686 | 0.3708 | 0.3729 | 0.3749 | 0.3770 | 0.3790 | 0.3810 | 0.3830 |
| 1.2 | 0.3849 | 0.3869 | 0.3888 | 0.3907 | 0.3925 | 0.3944 | 0.3962 | 0.3980 | 0.3997 | 0.4015 |
| 1.3 | 0.4032 | 0.4049 | 0.4066 | 0.4082 | 0.4099 | 0.4115 | 0.4131 | 0.4147 | 0.4162 | 0.4177 |
| 1.4 | 0.4192 | 0.4207 | 0.4222 | 0.4236 | 0.4251 | 0.4265 | 0.4279 | 0.4292 | 0.4306 | 0.4319 |
| 1.5 | 0.4332 | 0.4345 | 0.4357 | 0.4370 | 0.4382 | 0.4394 | 0.4406 | 0.4418 | 0.4429 | 0.4441 |
| 1.6 | 0.4452 | 0.4463 | 0.4474 | 0.4484 | 0.4495 | 0.4505 | 0.4515 | 0.4525 | 0.4535 | 0.4545 |
| 1.7 | 0.4554 | 0.4564 | 0.4573 | 0.4582 | 0.4591 | 0.4599 | 0.4608 | 0.4616 | 0.4625 | 0.4633 |
| 1.8 | 0.4641 | 0.4649 | 0.4656 | 0.4664 | 0.4671 | 0.4678 | 0.4686 | 0.4693 | 0.4699 | 0.4706 |
| 1.9 | 0.4713 | 0.4719 | 0.4726 | 0.4732 | 0.4738 | 0.4744 | 0.4750 | 0.4756 | 0.4761 | 0.4767 |
| 2.0 | 0.4772 | 0.4778 | 0.4783 | 0.4788 | 0.4793 | 0.4798 | 0.4803 | 0.4808 | 0.4812 | 0.4817 |
| 2.1 | 0.4821 | 0.4826 | 0.4830 | 0.4834 | 0.4838 | 0.4842 | 0.4846 | 0.4850 | 0.4854 | 0.4857 |
| 2.2 | 0.4861 | 0.4864 | 0.4868 | 0.4871 | 0.4875 | 0.4878 | 0.4881 | 0.4884 | 0.4887 | 0.4890 |
| 2.3 | 0.4893 | 0.4896 | 0.4898 | 0.4901 | 0.4904 | 0.4906 | 0.4909 | 0.4911 | 0.4913 | 0.4916 |
| 2.4 | 0.4918 | 0.4920 | 0.4922 | 0.4925 | 0.4927 | 0.4929 | 0.4931 | 0.4932 | 0.4934 | 0.4936 |
| 2.5 | 0.4938 | 0.4940 | 0.4941 | 0.4943 | 0.4945 | 0.4946 | 0.4948 | 0.4949 | 0.4951 | 0.4952 |
| 2.6 | 0.4953 | 0.4955 | 0.4956 | 0.4957 | 0.4959 | 0.4960 | 0.4961 | 0.4962 | 0.4963 | 0.4964 |
| 2.7 | 0.4965 | 0.4966 | 0.4967 | 0.4968 | 0.4969 | 0.4970 | 0.4971 | 0.4972 | 0.4973 | 0.4974 |
| 2.8 | 0.4974 | 0.4975 | 0.4976 | 0.4977 | 0.4977 | 0.4978 | 0.4979 | 0.4979 | 0.4980 | 0.4981 |
| 2.9 | 0.4981 | 0.4982 | 0.4982 | 0.4983 | 0.4984 | 0.4984 | 0.4985 | 0.4985 | 0.4986 | 0.4986 |
| 3.0 | 0.4987 | 0.4987 | 0.4987 | 0.4988 | 0.4988 | 0.4989 | 0.4989 | 0.4989 | 0.4990 | 0.4990 |
| 3.1 | 0.4990 | 0.4991 | 0.4991 | 0.4991 | 0.4992 | 0.4992 | 0.4992 | 0.4992 | 0.4993 | 0.4993 |
| 3.2 | 0.4993 | 0.4993 | 0.4994 | 0.4994 | 0.4994 | 0.4994 | 0.4994 | 0.4995 | 0.4995 | 0.4995 |
| 3.3 | 0.4995 | 0.4995 | 0.4995 | 0.4996 | 0.4996 | 0.4996 | 0.4996 | 0.4996 | 0.4996 | 0.4997 |
| 3.4 | 0.4997 | 0.4997 | 0.4997 | 0.4997 | 0.4997 | 0.4997 | 0.4997 | 0.4997 | 0.4997 | 0.4998 |
| 3.5 | 0.4998 | 0.4998 | 0.4998 | 0.4998 | 0.4998 | 0.4998 | 0.4998 | 0.4998 | 0.4998 | 0.4998 |
| 3.6 | 0.4998 | 0.4998 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 |
| 3.7 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 |
| 3.8 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 | 0.4999 |
| 3.9 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 |

The standard deviation is the square root of the average squared differences between the individual observations and the population mean:

$$\sigma = \sqrt{\frac{\sum_{i=1}^N (x_i - \mu)^2}{N}}$$

(2.11)

The standard deviation  $\sigma$  may be estimated by calculating the standard deviation  $s$  drawn from a small sample set as follows:

$$s = \sqrt{\frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N}} \quad \text{or} \quad s = \sqrt{\frac{x_1^2 + x_2^2 + \cdots - [(x_1 + x_2 + \cdots)^2]/N}{N - 1}} \quad (2.12)$$

where  $x_i - \bar{x}$  represents the deviation of each number in the array from the arithmetic mean. Since two pieces of information, namely  $s$  and  $\bar{x}$ , have been extracted from the data, we are left with  $N - 1$  *degrees of freedom* (df); that is, independent data points available for measurement of precision. If a relatively large sample of data corresponding to  $N > 30$  is available, its mean can be taken as a measure of  $\mu$ , and  $s$  as equal to  $\sigma$ .

So basic is the notion of a statistical *estimate* of a physical parameter that statisticians use Greek letters for the *parameters* and Latin letters for the estimates. For many purposes, one uses the *variance*, which for the sample is  $s^2$  and for the entire populations is  $\sigma^2$ . The variance  $s^2$  of a finite sample is an unbiased estimate of  $\sigma^2$ , whereas the standard deviation  $s$  is not an unbiased estimate of  $\sigma$ .

Because the standard deviation  $\sigma$  for the universe is a characteristic of the measuring procedure, it is possible to get a good estimate not only from a long series of repeated analyses of the same sample, but also by taking together several short series measured with slightly different samples of the same type. When a series of observations can be logically arranged into  $k$  subgroups, the variance is calculated by summing the squares of the deviations for each subgroup, and then adding all the  $k$  sums and dividing by  $N - k$  because one degree of freedom is lost in each subgroup. It is not required that the number of repeated analyses in the different groups be the same. For two groups of observations consisting of  $N_A$  and  $N_B$  members of standard deviations  $s_A$  and  $s_B$ , respectively, the variance is given by:

$$s^2 = \frac{(N_A - 1)s_A^2 + (N_B - 1)s_B^2}{N_A + N_B - 2} \quad (2.13)$$

Another measure of dispersion is the *coefficient of variation*, which is merely the standard deviation expressed as a fraction of the arithmetic mean, viz.,  $s/\bar{x}$ . It is useful mainly to show whether the relative or the absolute spread of values is constant as the values are changed.

### 2.3.6 Student's Distribution or $t$ Test

In the next several sections, the theoretical distributions and tests of significance will be examined beginning with Student's distribution or  $t$  test. If the data contained only random (or chance) errors, the cumulative estimates  $\bar{x}$  and  $s$  would gradually approach the limits  $\mu$  and  $\sigma$ . The distribution of results would be normally distributed with mean  $\mu$  and standard deviation  $\sigma$ . Were the true mean of the infinite population known, it would also have some symmetrical type of distribution centered around  $\mu$ . However, it would be expected that the dispersion or spread of this dispersion about the mean would depend on the sample size.

The standard deviation of the distribution of means equals  $\sigma/N^{1/2}$ . Since  $\sigma$  is not usually known, its approximation for a finite number of measurements is overcome by the Student  $t$  test. It is a measure of error between  $\mu$  and  $\bar{x}$ . The Student  $t$  takes into account both the possible variation of the value of  $\bar{x}$  from  $\mu$  on the basis of the expected variance  $\sigma^2/N^{1/2}$  and the reliability of using  $s$  in place of  $\sigma$ . The distribution of the statistic is:

$$\pm t = \frac{\bar{x} - \mu}{s/\sqrt{N}} \quad \text{or} \quad \mu = \bar{x} \pm \frac{ts}{\sqrt{N}} \quad (2.14)$$

The distribution of the  $t$ -statistic  $(\bar{x} - \mu)s$  is symmetrical about zero and is a function of the degrees of freedom. Limits assigned to the distance on either side of  $\mu$  are called *confidence limits*. The percentage probability that  $\mu$  lies within this interval is called the *confidence level*. The *level of significance* or *error probability* ( $100 - \text{confidence level}$  or  $100 - \alpha$ ) is the percent probability that  $\mu$  will lie outside the confidence interval, and represents the chances of being incorrect in stating that  $\mu$  lies within the confidence interval. Values of  $t$  are in Table 2.27 for any desired degrees of freedom and various confidence levels.

An analytical procedure is often tested on materials of known composition. These materials may be pure substances, standard samples, or materials analyzed by some other more accurate method. Repeated determinations on a known material furnish data for both an estimate of the precision and a test for the presence of a constant error in the results. The standard deviation is found from Equation 12 (with the known composition replacing  $\mu$ ). A calculated value for  $t$  (Eq. 14) in excess of the appropriate value in Table 2.27 is interpreted as evidence of the presence of a constant error at the indicated level of significance.

**TABLE 2.27** Percentile Values for Student  $t$  Distribution

| df       | $t_{0.995}$ | $t_{0.99}$ | $t_{0.975}$ | $t_{0.95}$ | $t_{0.90}$ | $t_{0.80}$ | $t_{0.75}$ | $t_{0.70}$ | $t_{0.60}$ | $t_{0.55}$ |
|----------|-------------|------------|-------------|------------|------------|------------|------------|------------|------------|------------|
| 1        | 63.66       | 31.82      | 12.71       | 6.31       | 3.08       | 1.376      | 1.000      | 0.727      | 0.325      | 0.158      |
| 2        | 9.92        | 6.96       | 4.30        | 2.92       | 1.89       | 1.061      | 0.816      | 0.617      | 0.289      | 0.142      |
| 3        | 5.84        | 4.54       | 3.18        | 2.35       | 1.64       | 0.978      | 0.765      | 0.584      | 0.277      | 0.137      |
| 4        | 4.60        | 3.75       | 2.78        | 2.13       | 1.53       | 0.941      | 0.741      | 0.569      | 0.271      | 0.134      |
| 5        | 4.03        | 3.36       | 2.57        | 2.02       | 1.48       | 0.920      | 0.727      | 0.559      | 0.267      | 0.132      |
| 6        | 3.71        | 3.14       | 2.45        | 1.94       | 1.44       | 0.906      | 0.718      | 0.553      | 0.265      | 0.131      |
| 7        | 3.50        | 3.00       | 2.36        | 1.90       | 1.42       | 0.896      | 0.711      | 0.549      | 0.263      | 0.130      |
| 8        | 3.36        | 2.90       | 2.31        | 1.86       | 1.40       | 0.889      | 0.706      | 0.546      | 0.262      | 0.130      |
| 9        | 3.25        | 2.82       | 2.26        | 1.83       | 1.38       | 0.883      | 0.703      | 0.543      | 0.261      | 0.129      |
| 10       | 3.17        | 2.76       | 2.23        | 1.81       | 1.37       | 0.879      | 0.700      | 0.542      | 0.260      | 0.129      |
| 11       | 3.11        | 2.72       | 2.20        | 1.80       | 1.36       | 0.876      | 0.697      | 0.540      | 0.260      | 0.129      |
| 12       | 3.06        | 2.68       | 2.18        | 1.78       | 1.36       | 0.873      | 0.695      | 0.539      | 0.259      | 0.128      |
| 13       | 3.01        | 2.65       | 2.16        | 1.77       | 1.35       | 0.870      | 0.694      | 0.538      | 0.259      | 0.128      |
| 14       | 2.98        | 2.62       | 2.14        | 1.76       | 1.34       | 0.868      | 0.692      | 0.537      | 0.258      | 0.128      |
| 15       | 2.95        | 2.60       | 2.13        | 1.75       | 1.34       | 0.866      | 0.691      | 0.536      | 0.258      | 0.128      |
| 16       | 2.92        | 2.58       | 2.12        | 1.75       | 1.34       | 0.865      | 0.690      | 0.535      | 0.258      | 0.128      |
| 17       | 2.90        | 2.57       | 2.11        | 1.74       | 1.33       | 0.863      | 0.689      | 0.534      | 0.257      | 0.128      |
| 18       | 2.88        | 2.55       | 2.10        | 1.73       | 1.33       | 0.862      | 0.688      | 0.534      | 0.257      | 0.127      |
| 19       | 2.86        | 2.54       | 2.09        | 1.73       | 1.33       | 0.861      | 0.688      | 0.533      | 0.257      | 0.127      |
| 20       | 2.84        | 2.53       | 2.09        | 1.72       | 1.32       | 0.860      | 0.687      | 0.533      | 0.257      | 0.127      |
| 21       | 2.83        | 2.52       | 2.08        | 1.72       | 1.32       | 0.859      | 0.686      | 0.532      | 0.257      | 0.127      |
| 22       | 2.82        | 2.51       | 2.07        | 1.72       | 1.32       | 0.858      | 0.686      | 0.532      | 0.256      | 0.127      |
| 23       | 2.81        | 2.50       | 2.07        | 1.71       | 1.32       | 0.858      | 0.685      | 0.532      | 0.256      | 0.127      |
| 24       | 2.80        | 2.49       | 2.06        | 1.71       | 1.32       | 0.857      | 0.685      | 0.531      | 0.256      | 0.127      |
| 25       | 2.79        | 2.48       | 2.06        | 1.71       | 1.32       | 0.856      | 0.684      | 0.531      | 0.256      | 0.127      |
| 26       | 2.78        | 2.48       | 2.06        | 1.71       | 1.32       | 0.856      | 0.684      | 0.531      | 0.256      | 0.127      |
| 27       | 2.77        | 2.47       | 2.05        | 1.70       | 1.31       | 0.855      | 0.684      | 0.531      | 0.256      | 0.127      |
| 28       | 2.76        | 2.47       | 2.05        | 1.70       | 1.31       | 0.855      | 0.683      | 0.530      | 0.256      | 0.127      |
| 29       | 2.76        | 2.46       | 2.04        | 1.70       | 1.31       | 0.854      | 0.683      | 0.530      | 0.256      | 0.127      |
| 30       | 2.75        | 2.46       | 2.04        | 1.70       | 1.31       | 0.854      | 0.683      | 0.530      | 0.256      | 0.127      |
| 40       | 2.70        | 2.42       | 2.02        | 1.68       | 1.30       | 0.851      | 0.681      | 0.529      | 0.255      | 0.126      |
| 60       | 2.66        | 2.39       | 2.00        | 1.67       | 1.30       | 0.848      | 0.679      | 0.527      | 0.254      | 0.126      |
| 120      | 2.62        | 2.36       | 2.98        | 1.66       | 1.29       | 0.845      | 0.677      | 0.526      | 0.254      | 0.126      |
| $\infty$ | 2.58        | 2.33       | 1.96        | 1.645      | 1.28       | 0.842      | 0.674      | 0.524      | 0.253      | 0.126      |

*Example 7* A new method for the analysis of iron using pure FeO was replicated with five samples giving these results (in % Fe): 76.95, 77.02, 76.90, 77.20, and 77.50. Does a systematic error exist?

From Equation 4,  $\bar{x}$  is 77.11; and from Equation 5,  $s$  is 0.24 for 4 degrees of freedom. Because  $\sigma$  is not known, the Student  $t_{0.975}$  (2.78 for 4 degrees of freedom) is used to calculate the confidence interval at the 95% probability level.

$$\mu = \bar{x} \pm \frac{ts}{\sqrt{N}} = 77.11 \pm \frac{(2.78)(0.24)}{\sqrt{5}} = 77.11 \pm 0.30$$

We used a two-tailed test. Upon rereading the problem, we realize that this was pure FeO whose iron content was 77.60% so that  $\mu = 77.60$  and the confidence interval does not include the known value. Since the FeO was a standard, a one-tailed test should have been used since only random values would be expected to exceed 77.60%. Now the Student  $t$  value of 2.13 (for  $-t_{0.05}$ ) should have been used, and now the confidence interval becomes  $77.11 \pm 0.23$ . A systematic error is presumed to exist.

The  $t$  test can be applied to differences between pairs of observations. Perhaps only a single pair can be performed at one time, or possibly one wishes to compare two methods using samples of differing analytical content. It is still necessary that the two methods possess the same inherent standard deviation. An average difference  $\bar{d}$  calculated, and individual deviations from  $\bar{d}$  are used to evaluate the variance of the differences.

*Example 8* From the following data do the two methods actually give concordant results?

| Sample | Method A | Method B | Difference       |
|--------|----------|----------|------------------|
| 1      | 33.27    | 33.04    | $d_1 = 0.23$     |
| 2      | 51.34    | 50.96    | $d_2 = 0.38$     |
| 3      | 23.91    | 23.77    | $d_3 = 0.14$     |
| 4      | 47.04    | 46.79    | $d_4 = 0.25$     |
|        |          |          | $\bar{d} = 0.25$ |

$$s_d = \frac{\sqrt{\sum (d - \bar{d})^2}}{N - 1} = 0.099$$
$$t = \frac{0.25}{0.099} \sqrt{4 - 1} = 4.30$$

From Table 2.27,  $t_{0.975} = 3.18$  (at 95% probability) and  $t_{0.995} = 5.84$  (at 99% probability). The difference between the two methods is probably significant.

If the  $t$ -value falls short of the formal significance level, this is not to be interpreted as proving the absence of a systematic error. Perhaps the data were insufficient in precision or in number to establish the presence of a constant error. Especially when the calculated value for  $t$  is only slightly short of the tabulated value, some additional data may suffice to build up the evidence for a constant error (or the lack thereof).

Should there be more than one known material, a weighted average of the individual differences ( $\bar{x}$ ) should be taken. The value of  $s$  should be based on the combined estimate from the two or more materials (perhaps different primary standards for bases). Should the materials differ markedly in composition, a plot of the individual constant errors against composition should be made. If the constant error appear to depend upon the composition, they should not be pooled in a weighted average.

The  $t$  test is also used to judge whether a given lot of material conforms to a particular specification. If both plus and minus departures from the known value are to be guarded against, a two-tailed test is involved. If departures in only one direction are undesirable, then the 10% level values for  $t$  are appropriate for the 5% level in *one* direction. Similarly, the 2% level should be used to obtain the 1% level to test the departure from the known value in one direction only; these constitute a one-tailed test. More on this subject will be in the next section.

Sometimes just one determination is available on each of several known materials similar in composition. A single determination by each of two procedures (or two analysts) on a series of material may be used to test for a relative bias between the two methods, as in Example 2.4. Of course, the average difference does not throw any light on which procedure has the larger constant error. It only supplies a test as to whether the two procedures are in disagreement.

### 2.3.7 Hypotheses About Means

Statistical methods are frequently used to give a “yes” or “no” answer to a particular question concerning the significance of data. When performing hypothesis tests on real data, we cannot set an absolute cutoff as to where we can expect to find no values from the population against which we are testing data, but we can set a limit beyond which we consider it very unlikely to find a member of the population. If a measurement is made that does in fact fall outside the specified range, the probability of its happening by chance alone can be rejected; something beyond the randomness of the reference population must be operating. In other words, hypothesis testing is an attempt to determine whether a given measured statistic could have come from some hypothesized population.

In attempting to reach decisions, it is useful to make assumptions or guesses about the populations involved. Such assumptions, which may or may not be true, are called *statistical hypotheses* and in general are statements about the probability distributions of the populations. A common procedure is to set up a *null hypothesis*, denoted by  $H_0$ , which states that there is no significant difference between two sets of data or that a variable exerts no significant effect. Any hypothesis which differs from a null hypothesis is called an *alternative hypothesis*, denoted by  $H_1$ .

Our answer is qualified by a confidence level (or level of significance) indicating the degree of certainty of the answer. Generally confidence levels of 95% and 99% are chosen to express the probability that the answer is correct. These are also denoted as the 0.05 and 0.01 level of significance, respectively. When the hypothesis can be rejected at the 0.05 level of significance, but not at the 0.01 level, we can say that the sample results are probably significant. If, however, the hypothesis is also rejected at the 0.01 level, the results become highly significant.

The abbreviated table on the next page, which gives critical values of  $z$  for both one-tailed and two-tailed tests at various levels of significance, will be found useful for purposes of reference. Critical values of  $z$  for other levels of significance are found by the use of Table 2.26b. For a small number of samples we replace  $z$ , obtained from above or from Table 2.26b, by  $t$  from Table 2.27, and we replace  $\sigma$  by:

$$[\sqrt{N/(N-1)}] s$$

| Level of significance, $\alpha$             | 0.10                 | 0.05                | 0.01               | 0.005              | 0.002              |
|---------------------------------------------|----------------------|---------------------|--------------------|--------------------|--------------------|
| Critical values of $z$ for one-tailed tests | – 1.28<br>or 1.28    | – 1.645<br>or 1.645 | – 2.33<br>or 2.33  | – 2.58<br>or 2.58  | – 2.88<br>or 2.88  |
| Critical values of $z$ for two-tailed tests | – 1.645<br>and 1.645 | – 1.96<br>and 1.96  | – 2.58<br>and 2.58 | – 2.81<br>and 2.81 | – 3.08<br>and 3.08 |

Procedures which enable us to decide whether to accept or reject hypotheses or to determine whether observed samples differ significantly from expected results are called *tests of hypotheses*, *tests of significance*, or *rules of decision*. For example, a set of  $z$  values outside the range – 1.96 to 1.96 (at the 0.05 level of significance for a two-tailed test), constitute what is called the critical region or region of rejection of the hypothesis. The set of  $z$  results inside the range – 1.96 to 1.96 could then be called the region of acceptance of the hypothesis.

*Example 9* In the past a method gave  $\mu = 0.050\%$ . A recent set of 10 results gave  $\bar{x} = 0.053\%$  and  $s = 0.003\%$ . Is everything satisfactory at a level of significance of 0.05? Of 0.01? We wish to decide between the hypotheses:

- $H_0: \mu = 0.050\%$       and the method is working properly, and
- $H_1: \mu \neq 0.050\%$       and the method is not working properly.

A *two-tailed test* is required; that is, both tails on the distribution curve are involved:

$$t = \frac{0.053 - 0.050}{0.003} \sqrt{10 - 1} = -3.00$$

Enter Table 2.27 for nine degrees of freedom under the column headed  $t_{0.975}$  for the 0.05 level of significance, and the column  $t_{0.995}$  for the 0.01 level of significance. At the 0.05 level, accept  $H_0$  if  $t$  lies inside the interval  $-t_{0.975}$  to  $t_{0.975}$ , that is, within – 2.26 and 2.26; reject otherwise. Since  $t = -3.00$ , we reject  $H_0$ . At the 0.01 level of significance, the corresponding interval is – 3.25 to 3.25, which  $t$  lies within, indicating acceptance of  $H_0$ . Because we can reject  $H_0$  at the 0.05 level but not at the 0.01 level of significance, we can say that the sample results are probably significant and that the method is working properly.

Let us digress a moment and consider when a two-tailed test is needed, and what a one-tailed test implies. We “assume” that the measurements can be described by the curve shown in Fig. 2.10. If so, then 95% of the time a sample from the specified population will fall within the indicated range and 5% of the time it will fall outside; 2.5% of the time it is outside on the high side of the range, and 2.5% of the time it is below the low side of the range. Our assumption implies that if  $\mu$  does not equal the hypothesized value, the probability of its being above the hypothesized value is equal to the probability of its being below the hypothesized value.

There will be incidences when the foregoing assumptions for a two-tailed test will not be true. Perhaps some physical situation prevents  $\mu$  from ever being less than the hypothesized value; it can only be equal or greater. No results would ever fall below the low end of the confidence interval; only the upper end of the distribution is operative. Now random samples will exceed the upper bound only 2.5% of the time, not the 5% specified in two-tail testing. Thus, where the possible values are restricted, what was supposed to be a hypothesis test at the 95% confidence level is actually being performed at a 97.5% confidence level. Stated in another way, 95% of the population data lie within the interval below  $\mu + 1.65\sigma$  and 5% lie above. Of course, the opposite situation might also occur and only the lower end of the distribution is operative.

**Example 10** Six samples from a bulk chemical shipment averaged 77.50% active ingredient with  $s = 1.45\%$ . The manufacturer claimed 80.00%. Can this claim be supported?

A one-tailed test is required since the alternative hypothesis states that the population parameter is equal to or less than the hypothesized value.

$$t = \frac{77.50 - 80.00}{1.45} \sqrt{6 - 1} = 3.86$$

Since  $t_{0.95} = -2.01$ , and  $t_{0.99} = -3.36$ , the hypothesis is rejected at both the 0.05 and the 0.01 levels of significance. It is extremely unlikely that the claim is justified.

### 2.3.8 The Chi-square ( $\chi^2$ ) Distribution

The  $\chi^2$  distribution describes the behavior of variances. Actually there is not a single  $\chi^2$  distribution but a whole set of distributions. Each distribution depends upon the number of degrees of freedom (designated variously as  $df$ ,  $d.f.$ , or  $f$ ) in that distribution. Table 2.28 is laid out so that the horizontal axis is labeled with probability levels, while the vertical axis is listed in descending order of increasing number of degrees of freedom. The entries increase both as you read down and across the table. Although Table 2.28 does not display the values for the mid-range of the distributions, at the 50% point of each distribution, the expected value of  $\chi^2$  is equal to the degrees of freedom. Estimates of the variance are uncertain when based only on a few degrees of freedom. With the 10 samples in Example 11, the standard deviation can vary by a large factor purely by random chance alone. Even 31 samples gives a spread of standard deviation of 2.6 at the 95% confidence level.

Understanding the  $\chi^2$  distribution allows us to calculate the expected values of random variables that are normally and independently distributed. In least squares multiple regression, or in calibration work in general, there is a basic assumption that the error in the response variable is random and normally distributed, with a variance that follows a  $\chi^2$  distribution.

Confidence limits for an estimate of the variance may be calculated as follows. For each group of samples a standard deviation is calculated. These estimates of  $\sigma$  possess a distribution called the  $\chi^2$  distribution:

$$\chi^2 = \frac{s^2}{\sigma^2/df} \quad (2.15)$$

The upper and lower confidence limits for the standard deviation are obtained by dividing  $(N - 1)s^2$  by two entries taken from Table 2.28. The estimate of variance at the 90% confidence limits is for use in the entries  $\chi_{0.05}^2$  and  $\chi_{0.95}^2$  (for 5% and 95%) with  $N$  degrees of freedom.

**Example 11** The variance obtained for 10 samples is  $(0.65)^2$ .  $\sigma^2$  is known to be  $(0.75)^2$ . How reliable is  $s^2$  as an estimate of  $\sigma^2$ ?

$$\begin{aligned} \frac{s^2 (N - 1)}{\chi_{0.975}^2} &< \sigma^2 < \frac{s^2 (N - 1)}{\chi_{0.025}^2} \\ \frac{(0.65)^2 (10 - 1)}{19.02} &< \sigma^2 < \frac{(0.65)^2 (10 - 1)}{2.70} \\ 0.20 &< \sigma^2 < 1.43 \end{aligned}$$

Thus, only one time in 40 will  $9s^2/\sigma^2$  be less than 2.70 by chance alone. Similarly, only one time



**TABLE 2.28** Percentile Values for the Chi-square ( $\chi^2$ ) Distribution

| df  | $\chi^2_{0.995}$ | $\chi^2_{0.99}$ | $\chi^2_{0.975}$ | $\chi^2_{0.95}$ | $\chi^2_{0.90}$ | $\chi^2_{0.75}$ | $\chi^2_{0.50}$ | $\chi^2_{0.25}$ | $\chi^2_{0.10}$ | $\chi^2_{0.05}$ | $\chi^2_{0.025}$ | $\chi^2_{0.01}$ | $\chi^2_{0.005}$ |
|-----|------------------|-----------------|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|------------------|-----------------|------------------|
| 1   | 7.88             | 6.63            | 5.02             | 3.84            | 2.71            | 1.32            | 0.455           | 0.102           | 0.0158          | 0.0039          | 0.0010           | 0.0002          | 0.0000           |
| 2   | 10.6             | 9.21            | 7.38             | 5.99            | 4.61            | 2.77            | 1.39            | 0.575           | 0.211           | 0.103           | 0.0506           | 0.0201          | 0.0100           |
| 3   | 12.8             | 11.3            | 9.35             | 7.81            | 6.25            | 4.11            | 2.37            | 1.21            | 0.584           | 0.352           | 0.216            | 0.115           | 0.072            |
| 4   | 14.9             | 13.3            | 11.1             | 9.49            | 7.78            | 5.39            | 3.36            | 1.92            | 1.06            | 0.711           | 0.484            | 0.297           | 0.207            |
| 5   | 16.7             | 15.1            | 12.8             | 11.1            | 9.24            | 6.63            | 4.35            | 2.67            | 1.61            | 1.15            | 0.831            | 0.554           | 0.412            |
| 6   | 18.5             | 16.8            | 14.4             | 12.6            | 10.6            | 7.84            | 5.35            | 3.45            | 2.20            | 1.64            | 1.24             | 0.872           | 0.676            |
| 7   | 20.3             | 18.5            | 16.0             | 14.1            | 12.0            | 9.04            | 6.35            | 4.25            | 2.83            | 2.17            | 1.69             | 1.24            | 0.989            |
| 8   | 22.0             | 20.1            | 17.5             | 15.5            | 13.4            | 10.2            | 7.34            | 5.07            | 3.49            | 2.73            | 2.18             | 1.65            | 1.34             |
| 9   | 23.6             | 21.7            | 19.0             | 16.9            | 14.7            | 11.4            | 8.34            | 5.90            | 4.17            | 3.33            | 2.70             | 2.09            | 1.73             |
| 10  | 25.2             | 23.2            | 20.5             | 18.3            | 16.0            | 12.5            | 9.34            | 6.74            | 4.87            | 3.94            | 3.25             | 2.56            | 2.16             |
| 11  | 26.8             | 24.7            | 21.9             | 19.7            | 17.3            | 13.7            | 10.3            | 7.58            | 5.58            | 4.57            | 3.82             | 3.05            | 2.60             |
| 12  | 28.3             | 26.2            | 23.3             | 21.0            | 18.5            | 14.8            | 11.3            | 8.44            | 6.30            | 5.23            | 4.40             | 3.57            | 3.07             |
| 13  | 29.8             | 27.7            | 24.7             | 22.4            | 19.8            | 16.0            | 12.3            | 9.30            | 7.04            | 5.89            | 5.01             | 4.11            | 3.57             |
| 14  | 31.3             | 29.1            | 26.1             | 23.7            | 21.1            | 17.1            | 13.3            | 10.2            | 7.79            | 6.57            | 5.63             | 4.66            | 4.07             |
| 15  | 32.8             | 30.6            | 27.5             | 25.0            | 22.3            | 18.2            | 14.3            | 11.0            | 8.55            | 7.26            | 6.26             | 5.23            | 4.60             |
| 16  | 34.3             | 32.0            | 28.8             | 26.3            | 23.5            | 19.4            | 15.3            | 11.9            | 9.31            | 7.96            | 6.91             | 5.81            | 5.14             |
| 17  | 35.7             | 33.4            | 30.2             | 27.6            | 24.8            | 20.5            | 16.3            | 12.8            | 10.1            | 8.67            | 7.56             | 6.41            | 5.70             |
| 18  | 37.2             | 34.8            | 31.5             | 28.9            | 26.0            | 21.6            | 17.3            | 13.7            | 10.9            | 9.39            | 8.23             | 7.01            | 6.26             |
| 19  | 38.6             | 36.2            | 32.9             | 30.1            | 27.2            | 22.7            | 18.3            | 14.6            | 11.7            | 10.1            | 8.91             | 7.63            | 6.84             |
| 20  | 40.0             | 37.6            | 34.2             | 31.4            | 28.4            | 23.8            | 19.3            | 15.5            | 12.4            | 10.9            | 9.59             | 8.26            | 7.43             |
| 21  | 41.4             | 38.9            | 35.5             | 32.7            | 29.6            | 24.9            | 20.3            | 16.3            | 13.2            | 11.6            | 10.3             | 8.90            | 8.03             |
| 22  | 42.8             | 40.3            | 36.8             | 33.9            | 30.8            | 26.0            | 21.3            | 17.2            | 14.0            | 12.3            | 11.0             | 9.54            | 8.64             |
| 23  | 44.2             | 41.6            | 38.1             | 35.2            | 32.0            | 27.1            | 22.3            | 18.1            | 14.8            | 13.1            | 11.7             | 10.2            | 9.26             |
| 24  | 45.6             | 43.0            | 39.4             | 36.4            | 33.2            | 28.2            | 23.3            | 19.0            | 15.7            | 13.8            | 12.4             | 10.9            | 9.89             |
| 25  | 46.9             | 44.3            | 40.6             | 37.7            | 34.4            | 29.3            | 24.3            | 19.9            | 16.5            | 14.6            | 13.1             | 11.5            | 10.5             |
| 26  | 48.3             | 45.6            | 41.9             | 38.9            | 35.6            | 30.4            | 25.3            | 20.8            | 17.3            | 15.4            | 13.8             | 12.2            | 11.2             |
| 27  | 49.6             | 47.0            | 43.2             | 40.1            | 36.7            | 31.5            | 26.3            | 21.7            | 18.1            | 16.2            | 14.6             | 12.9            | 11.8             |
| 28  | 51.0             | 48.3            | 44.5             | 41.3            | 37.9            | 32.6            | 27.3            | 22.7            | 18.9            | 16.9            | 15.39            | 13.6            | 12.5             |
| 29  | 52.3             | 49.6            | 45.7             | 42.6            | 39.1            | 33.7            | 28.3            | 23.6            | 19.8            | 17.7            | 16.0             | 14.3            | 13.1             |
| 30  | 53.7             | 50.9            | 47.0             | 43.8            | 40.3            | 34.8            | 29.3            | 24.5            | 20.6            | 18.5            | 16.8             | 15.0            | 13.8             |
| 40  | 66.8             | 63.7            | 59.3             | 55.8            | 51.8            | 45.6            | 39.3            | 33.7            | 29.1            | 26.5            | 24.4             | 22.2            | 20.7             |
| 50  | 79.5             | 76.2            | 71.4             | 67.5            | 63.2            | 56.3            | 49.3            | 42.9            | 37.7            | 34.8            | 32.4             | 29.7            | 28.0             |
| 60  | 92.0             | 88.4            | 83.3             | 79.1            | 74.4            | 67.0            | 59.3            | 52.3            | 46.5            | 43.2            | 40.5             | 37.5            | 35.5             |
| 70  | 104.2            | 100.4           | 95.0             | 90.5            | 85.5            | 77.6            | 69.3            | 61.7            | 55.3            | 51.7            | 48.8             | 45.4            | 43.3             |
| 80  | 116.3            | 112.3           | 106.6            | 101.9           | 96.6            | 88.1            | 79.3            | 71.1            | 64.3            | 60.4            | 57.2             | 53.5            | 51.2             |
| 90  | 128.3            | 124.1           | 118.1            | 113.1           | 107.6           | 98.6            | 89.3            | 80.6            | 73.3            | 69.1            | 65.6             | 61.8            | 59.2             |
| 100 | 140.2            | 135.8           | 129.6            | 124.3           | 118.5           | 109.1           | 99.3            | 90.1            | 82.4            | 77.9            | 74.2             | 70.1            | 67.3             |

in 40 will  $9s^2/\sigma^2$  be greater than 19.02. Consequently, it is not unlikely that  $s^2$  is a reliable estimate of  $\sigma^2$ .

Stated differently:

Upper limit:  $\sigma^2 = 9s^2/2.7 = 3.3s^2$

Lower limit:  $\sigma^2 = 9s^2/19.02 = 0.48s^2$

Ten measurements give an estimate of  $\sigma^2$  that may be as much as 3.3 times or only about one-half the true variance.

### 2.3.9 The $F$ Statistic

The  $F$  statistic, along with the  $z$ ,  $t$ , and  $\chi^2$  statistics, constitute the group that are thought of as fundamental statistics. Collectively they describe all the relationships that can exist between means and standard deviations. To perform an  $F$  test, we must first verify the randomness and independence of the errors. If  $\sigma_1^2 = \sigma_2^2$ , then  $s_1^2/s_2^2$  will be distributed properly as the  $F$  statistic. If the calculated  $F$  is outside the confidence interval chosen for that statistic, then this is evidence that  $\sigma_1^2 \neq \sigma_2^2$ .

The  $F$  statistic describes the distribution of the ratios of variances of two sets of samples. It requires three table labels: the probability level and the two degrees of freedom. Since the  $F$  distribution requires a three-dimensional table which is effectively unknown, the  $F$  tables are presented as large sets of two-dimensional tables. The  $F$  distribution in Table 2.29 has the different numbers of degrees of freedom for the denominator variance placed along the vertical axis, while in each table the two horizontal axes represent the numerator degrees of freedom and the probability level. Only two probability levels are given in Table 2.29: the upper 5% points ( $F_{0.95}$ ) and the upper 1% points ( $F_{0.99}$ ). More extensive tables of statistics will list additional probability levels, and they should be consulted when needed.

It is possible to compare the means of two relatively small sets of observations when the variances within the sets can be regarded as the same, as indicated by the  $F$  test. One can consider the distribution involving estimates of the true variance. With  $s_1^2$  determined from a group of  $N_1$  observations and  $s_2^2$  from a second group of  $N_2$  observations, the distribution of the ratio of the sample variances is given by the  $F$  statistic:

$$F = \frac{s_1^2/\sigma_1^2}{s_2^2/\sigma_2^2} \quad (2.16)$$

The larger variance is placed in the numerator. For example, the  $F$  test allows judgment regarding the existence of a significant difference in the precision between two sets of data or between two analysts. The hypothesis assumed is that both variances are indeed alike and a measure of the same  $\sigma$ .

The fact that each sample variance is related to its own population variance means that the sample variance being used for the calculation need not come from the same population. This is a significant departure from the assumptions inherent in the  $z$ ,  $t$ , and  $\chi^2$  statistics.

**Example 12** Suppose Analyst A made five observations and obtained a standard deviation of 0.06, where Analyst B with six observations obtained  $s_B = 0.03$ . The experimental variance ratio is:

$$F = \frac{(0.06)^2}{(0.03)^2} = 4.00$$

From Table 2.28 with four degrees of freedom for A and five degrees of freedom for B, the value of  $F$  would exceed 5.19 five percent of the time. Therefore, the null hypothesis is valid, and comparable skills are exhibited by the two analysts.

As applied in Example 12, the  $F$  test was one-tailed. The  $F$  test may also be applied as a two-tailed test in which the alternative to the null hypothesis is  $\sigma_1^2 \neq \sigma_2^2$ . This doubles the probability that the null hypothesis is invalid and has the effect of changing the confidence level, in the above example, from 95% to 90%.

If improvement in precision is claimed for a set of measurements, the variance for the set against which comparison is being made should be placed in the numerator, regardless of magnitude. An experimental  $F$  smaller than unity indicates that the claim for improved precision cannot be supported. The technique just given for examining whether the precision varies with the two different analytical procedures, also serves to compare the precision with different materials, or with different operators, laboratories, or sets of equipment.

**TABLE 2.29** *F* Distribution  
*Interpolation should be performed using reciprocals of the degrees of freedom.*

| Upper 5% points ( $F_{0.95}$ )     |                                  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |          |  |
|------------------------------------|----------------------------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|----------|--|
| Degrees of freedom for denominator | Degrees of freedom for numerator |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |          |  |
|                                    | 1                                | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   | 12   | 15   | 20   | 24   | 30   | 40   | 60   | 120  | $\infty$ |  |
| 1                                  | 161                              | 200  | 216  | 225  | 230  | 234  | 237  | 239  | 241  | 242  | 244  | 246  | 248  | 249  | 250  | 251  | 252  | 253  | 254      |  |
| 2                                  | 18.5                             | 19.0 | 19.2 | 19.2 | 19.3 | 19.3 | 19.4 | 19.4 | 19.4 | 19.4 | 19.4 | 19.4 | 19.4 | 19.5 | 19.5 | 19.5 | 19.5 | 19.5 | 19.5     |  |
| 3                                  | 10.1                             | 9.55 | 9.28 | 9.12 | 9.01 | 8.94 | 8.89 | 8.85 | 8.81 | 8.79 | 8.74 | 8.70 | 8.66 | 8.64 | 8.62 | 8.59 | 8.57 | 8.55 | 8.53     |  |
| 4                                  | 7.71                             | 6.94 | 6.59 | 6.39 | 6.26 | 6.16 | 6.09 | 6.04 | 6.00 | 5.96 | 5.91 | 5.86 | 5.80 | 5.77 | 5.75 | 5.72 | 5.69 | 5.66 | 5.63     |  |
| 5                                  | 6.61                             | 5.79 | 5.41 | 5.19 | 5.05 | 4.95 | 4.88 | 4.82 | 4.77 | 4.74 | 4.68 | 4.62 | 4.56 | 4.53 | 4.50 | 4.46 | 4.43 | 4.40 | 4.37     |  |
| 6                                  | 5.99                             | 5.14 | 4.76 | 4.53 | 4.39 | 4.28 | 4.21 | 4.15 | 4.10 | 4.06 | 4.00 | 3.94 | 3.87 | 3.84 | 3.81 | 3.77 | 3.74 | 3.70 | 3.67     |  |
| 7                                  | 5.59                             | 4.74 | 4.35 | 4.12 | 3.97 | 3.87 | 3.79 | 3.73 | 3.68 | 3.64 | 3.57 | 3.51 | 3.44 | 3.41 | 3.38 | 3.34 | 3.30 | 3.27 | 3.23     |  |
| 8                                  | 5.32                             | 4.46 | 4.07 | 3.84 | 3.69 | 3.58 | 3.50 | 3.44 | 3.39 | 3.35 | 3.28 | 3.22 | 3.15 | 3.12 | 3.08 | 3.04 | 3.01 | 2.97 | 2.93     |  |
| 9                                  | 5.12                             | 4.26 | 3.86 | 3.63 | 3.48 | 3.37 | 3.29 | 3.23 | 3.18 | 3.14 | 3.07 | 3.01 | 2.94 | 2.90 | 2.86 | 2.83 | 2.79 | 2.75 | 2.71     |  |
| 10                                 | 4.96                             | 4.10 | 3.71 | 3.48 | 3.33 | 3.22 | 3.14 | 3.07 | 3.02 | 2.98 | 2.91 | 2.85 | 2.77 | 2.74 | 2.70 | 2.66 | 2.62 | 2.58 | 2.54     |  |
| 11                                 | 4.84                             | 3.98 | 3.59 | 3.36 | 3.20 | 3.09 | 3.01 | 2.95 | 2.90 | 2.85 | 2.79 | 2.72 | 2.65 | 2.61 | 2.57 | 2.53 | 2.49 | 2.45 | 2.40     |  |
| 12                                 | 4.75                             | 3.89 | 3.49 | 3.26 | 3.11 | 3.00 | 2.91 | 2.85 | 2.80 | 2.75 | 2.69 | 2.62 | 2.54 | 2.51 | 2.47 | 2.43 | 2.38 | 2.34 | 2.30     |  |
| 13                                 | 4.67                             | 3.81 | 3.41 | 3.18 | 3.03 | 2.92 | 2.83 | 2.77 | 2.71 | 2.67 | 2.60 | 2.53 | 2.46 | 2.42 | 2.38 | 2.34 | 2.30 | 2.25 | 2.21     |  |
| 14                                 | 4.60                             | 3.74 | 3.34 | 3.11 | 2.96 | 2.85 | 2.76 | 2.70 | 2.65 | 2.60 | 2.53 | 2.46 | 2.39 | 2.35 | 2.31 | 2.27 | 2.22 | 2.18 | 2.13     |  |
| 15                                 | 4.54                             | 3.68 | 3.29 | 3.06 | 2.90 | 2.79 | 2.71 | 2.64 | 2.59 | 2.54 | 2.48 | 2.40 | 2.33 | 2.29 | 2.25 | 2.20 | 2.16 | 2.11 | 2.07     |  |
| 16                                 | 4.49                             | 3.63 | 3.24 | 3.01 | 2.85 | 2.74 | 2.66 | 2.59 | 2.54 | 2.49 | 2.42 | 2.35 | 2.28 | 2.24 | 2.19 | 2.15 | 2.11 | 2.06 | 2.01     |  |
| 17                                 | 4.45                             | 3.59 | 3.20 | 2.96 | 2.81 | 2.70 | 2.61 | 2.55 | 2.49 | 2.45 | 2.38 | 2.31 | 2.23 | 2.19 | 2.15 | 2.10 | 2.06 | 2.01 | 1.96     |  |
| 18                                 | 4.41                             | 3.55 | 3.16 | 2.93 | 2.77 | 2.66 | 2.58 | 2.51 | 2.46 | 2.41 | 2.34 | 2.27 | 2.19 | 2.15 | 2.11 | 2.06 | 2.02 | 1.97 | 1.92     |  |
| 19                                 | 4.38                             | 3.52 | 3.13 | 2.90 | 2.74 | 2.63 | 2.54 | 2.48 | 2.42 | 2.38 | 2.31 | 2.23 | 2.16 | 2.11 | 2.07 | 2.03 | 1.98 | 1.93 | 1.88     |  |
| 20                                 | 4.35                             | 3.49 | 3.10 | 2.87 | 2.71 | 2.60 | 2.51 | 2.45 | 2.39 | 2.35 | 2.28 | 2.20 | 2.12 | 2.08 | 2.04 | 1.99 | 1.95 | 1.90 | 1.84     |  |
| 21                                 | 4.32                             | 3.47 | 3.07 | 2.84 | 2.68 | 2.57 | 2.49 | 2.42 | 2.37 | 2.32 | 2.25 | 2.18 | 2.10 | 2.05 | 2.01 | 1.96 | 1.92 | 1.87 | 1.81     |  |
| 22                                 | 4.30                             | 3.44 | 3.05 | 2.82 | 2.66 | 2.55 | 2.46 | 2.40 | 2.34 | 2.30 | 2.23 | 2.15 | 2.07 | 2.03 | 1.98 | 1.94 | 1.89 | 1.84 | 1.78     |  |
| 23                                 | 4.28                             | 3.42 | 3.03 | 2.80 | 2.64 | 2.53 | 2.44 | 2.37 | 2.32 | 2.27 | 2.20 | 2.13 | 2.05 | 2.01 | 1.96 | 1.91 | 1.86 | 1.81 | 1.76     |  |
| 24                                 | 4.26                             | 3.40 | 3.01 | 2.78 | 2.62 | 2.51 | 2.42 | 2.36 | 2.30 | 2.25 | 2.18 | 2.11 | 2.03 | 1.98 | 1.94 | 1.89 | 1.84 | 1.79 | 1.73     |  |
| 25                                 | 4.24                             | 3.39 | 2.99 | 2.76 | 2.60 | 2.49 | 2.40 | 2.34 | 2.28 | 2.24 | 2.16 | 2.09 | 2.01 | 1.96 | 1.92 | 1.87 | 1.82 | 1.77 | 1.71     |  |
| 30                                 | 4.17                             | 3.32 | 2.92 | 2.69 | 2.53 | 2.42 | 2.33 | 2.27 | 2.21 | 2.16 | 2.09 | 2.01 | 1.93 | 1.89 | 1.84 | 1.79 | 1.74 | 1.68 | 1.62     |  |
| 40                                 | 4.08                             | 3.23 | 2.84 | 2.61 | 2.45 | 2.34 | 2.25 | 2.18 | 2.12 | 2.08 | 2.00 | 1.92 | 1.84 | 1.79 | 1.74 | 1.69 | 1.64 | 1.58 | 1.51     |  |
| 60                                 | 4.00                             | 3.15 | 2.76 | 2.53 | 2.37 | 2.25 | 2.17 | 2.10 | 2.04 | 1.99 | 1.92 | 1.84 | 1.75 | 1.70 | 1.65 | 1.59 | 1.53 | 1.47 | 1.39     |  |
| 120                                | 3.92                             | 3.07 | 2.68 | 2.45 | 2.29 | 2.18 | 2.09 | 2.02 | 1.96 | 1.91 | 1.83 | 1.75 | 1.66 | 1.61 | 1.55 | 1.50 | 1.43 | 1.35 | 1.25     |  |
| $\infty$                           | 3.84                             | 3.00 | 2.60 | 2.37 | 2.21 | 2.10 | 2.01 | 1.94 | 1.88 | 1.83 | 1.75 | 1.67 | 1.57 | 1.52 | 1.46 | 1.39 | 1.32 | 1.22 | 1.00     |  |

**TABLE 2.29** *F* Distribution (Continued)

|                                    | Upper 1% points ( $F_{0.99}$ )   |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |          |  |
|------------------------------------|----------------------------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|----------|--|
| Degrees of freedom for denominator | Degrees of freedom for numerator |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |          |  |
|                                    | 1                                | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   | 12   | 15   | 20   | 24   | 30   | 40   | 60   | 120  | $\infty$ |  |
| 1                                  | 4052                             | 5000 | 5403 | 5625 | 5764 | 5859 | 5928 | 5982 | 6023 | 6056 | 6106 | 6157 | 6209 | 6235 | 6261 | 6287 | 6313 | 6339 | 6366     |  |
| 2                                  | 98.5                             | 99.0 | 99.2 | 99.2 | 99.3 | 99.3 | 99.4 | 99.4 | 99.4 | 99.4 | 99.4 | 99.4 | 99.4 | 99.5 | 99.5 | 99.5 | 99.5 | 99.5 | 99.5     |  |
| 3                                  | 34.1                             | 30.8 | 29.5 | 28.7 | 28.2 | 27.9 | 27.7 | 27.5 | 27.3 | 27.2 | 27.1 | 26.9 | 26.7 | 26.6 | 26.5 | 26.4 | 26.3 | 26.2 | 26.1     |  |
| 4                                  | 21.2                             | 18.0 | 16.7 | 16.0 | 15.5 | 15.2 | 15.0 | 14.8 | 14.7 | 14.5 | 14.4 | 14.2 | 14.0 | 13.9 | 13.8 | 13.7 | 13.7 | 13.6 | 13.5     |  |
| 5                                  | 16.3                             | 13.3 | 12.1 | 11.4 | 11.0 | 10.7 | 10.5 | 10.3 | 10.2 | 10.1 | 9.89 | 9.72 | 9.55 | 9.47 | 9.38 | 9.29 | 9.20 | 9.11 | 9.02     |  |
| 6                                  | 13.7                             | 10.9 | 9.78 | 9.15 | 8.75 | 8.47 | 8.26 | 8.10 | 7.98 | 7.87 | 7.72 | 7.56 | 7.40 | 7.31 | 7.23 | 7.14 | 7.06 | 6.97 | 6.88     |  |
| 7                                  | 12.2                             | 9.55 | 8.45 | 7.85 | 7.46 | 7.19 | 6.99 | 6.84 | 6.72 | 6.62 | 6.47 | 6.31 | 6.16 | 6.07 | 5.99 | 5.91 | 5.82 | 5.74 | 5.65     |  |
| 8                                  | 11.3                             | 8.65 | 7.59 | 7.01 | 6.63 | 6.37 | 6.18 | 6.03 | 5.91 | 5.81 | 5.67 | 5.52 | 5.36 | 5.28 | 5.20 | 5.12 | 5.03 | 4.95 | 4.86     |  |
| 9                                  | 10.6                             | 8.02 | 6.99 | 6.42 | 6.06 | 5.80 | 5.61 | 5.47 | 5.35 | 5.26 | 5.11 | 4.96 | 4.81 | 4.73 | 4.65 | 4.57 | 4.48 | 4.40 | 4.31     |  |
| 10                                 | 10.0                             | 7.56 | 6.55 | 5.99 | 5.64 | 5.39 | 5.20 | 5.06 | 4.94 | 4.85 | 4.71 | 4.56 | 4.41 | 4.33 | 4.25 | 4.17 | 4.08 | 4.00 | 3.91     |  |
| 11                                 | 9.65                             | 7.21 | 6.22 | 5.67 | 5.32 | 5.07 | 4.89 | 4.74 | 4.63 | 4.54 | 4.40 | 4.25 | 4.10 | 4.02 | 3.94 | 3.86 | 3.78 | 3.69 | 3.60     |  |
| 12                                 | 9.33                             | 6.93 | 5.95 | 5.41 | 5.06 | 4.82 | 4.64 | 4.50 | 4.39 | 4.30 | 4.16 | 4.01 | 3.86 | 3.78 | 3.70 | 3.62 | 3.54 | 3.45 | 3.36     |  |
| 13                                 | 9.07                             | 6.70 | 5.74 | 5.21 | 4.86 | 4.62 | 4.44 | 4.30 | 4.19 | 4.10 | 3.96 | 3.82 | 3.66 | 3.59 | 3.51 | 3.43 | 3.34 | 3.25 | 3.17     |  |
| 14                                 | 8.86                             | 6.51 | 5.56 | 5.04 | 4.70 | 4.46 | 4.28 | 4.14 | 4.03 | 3.94 | 3.80 | 3.66 | 3.51 | 3.43 | 3.35 | 3.27 | 3.18 | 3.09 | 3.00     |  |
| 15                                 | 8.68                             | 6.36 | 5.42 | 4.89 | 4.56 | 4.32 | 4.14 | 4.00 | 3.89 | 3.80 | 3.67 | 3.52 | 3.37 | 3.29 | 3.21 | 3.13 | 3.05 | 2.96 | 2.87     |  |
| 16                                 | 8.53                             | 6.23 | 5.29 | 4.77 | 4.44 | 4.20 | 4.03 | 3.89 | 3.78 | 3.69 | 3.55 | 3.41 | 3.26 | 3.18 | 3.10 | 3.02 | 2.93 | 2.84 | 2.75     |  |
| 17                                 | 8.40                             | 6.11 | 5.19 | 4.67 | 4.34 | 4.10 | 3.93 | 3.79 | 3.68 | 3.59 | 3.46 | 3.31 | 3.16 | 3.08 | 3.00 | 2.92 | 2.83 | 2.75 | 2.65     |  |
| 18                                 | 8.29                             | 6.01 | 5.09 | 4.58 | 4.25 | 4.01 | 3.84 | 3.71 | 3.60 | 3.51 | 3.37 | 3.23 | 3.08 | 3.00 | 2.92 | 2.84 | 2.75 | 2.66 | 2.57     |  |
| 19                                 | 8.19                             | 5.93 | 5.01 | 4.50 | 4.17 | 3.94 | 3.77 | 3.63 | 3.52 | 3.43 | 3.30 | 3.15 | 3.00 | 2.92 | 2.84 | 2.76 | 2.67 | 2.58 | 2.49     |  |
| 20                                 | 8.10                             | 5.85 | 4.94 | 4.43 | 4.10 | 3.87 | 3.70 | 3.56 | 3.46 | 3.37 | 3.23 | 3.09 | 2.94 | 2.86 | 2.78 | 2.69 | 2.61 | 2.52 | 2.42     |  |
| 21                                 | 8.02                             | 5.78 | 4.87 | 4.37 | 4.04 | 3.81 | 3.64 | 3.51 | 3.40 | 3.31 | 3.17 | 3.03 | 2.88 | 2.80 | 2.72 | 2.64 | 2.55 | 2.46 | 2.36     |  |
| 22                                 | 7.95                             | 5.72 | 4.82 | 4.31 | 3.99 | 3.76 | 3.59 | 3.45 | 3.35 | 3.26 | 3.12 | 2.98 | 2.83 | 2.75 | 2.67 | 2.58 | 2.50 | 2.40 | 2.31     |  |
| 23                                 | 7.88                             | 5.66 | 4.76 | 4.26 | 3.94 | 3.71 | 3.54 | 3.41 | 3.30 | 3.21 | 3.07 | 2.93 | 2.78 | 2.70 | 2.62 | 2.54 | 2.45 | 2.35 | 2.26     |  |
| 24                                 | 7.82                             | 5.61 | 4.72 | 4.22 | 3.90 | 3.67 | 3.50 | 3.36 | 3.26 | 3.17 | 3.03 | 2.89 | 2.74 | 2.66 | 2.58 | 2.49 | 2.40 | 2.31 | 2.21     |  |
| 25                                 | 7.77                             | 5.57 | 4.68 | 4.18 | 3.86 | 3.63 | 3.46 | 3.32 | 3.22 | 3.13 | 2.99 | 2.85 | 2.70 | 2.62 | 2.53 | 2.45 | 2.36 | 2.27 | 2.17     |  |
| 30                                 | 7.56                             | 5.39 | 4.51 | 4.02 | 3.70 | 3.47 | 3.30 | 3.17 | 3.07 | 2.98 | 2.84 | 2.70 | 2.55 | 2.47 | 2.39 | 2.30 | 2.21 | 2.11 | 2.01     |  |
| 40                                 | 7.31                             | 5.18 | 4.31 | 3.83 | 3.51 | 3.29 | 3.12 | 2.99 | 2.89 | 2.80 | 2.66 | 2.52 | 2.37 | 2.29 | 2.20 | 2.11 | 2.02 | 1.92 | 1.80     |  |
| 60                                 | 7.08                             | 4.98 | 4.13 | 3.65 | 3.34 | 3.12 | 2.95 | 2.82 | 2.72 | 2.63 | 2.50 | 2.35 | 2.20 | 2.12 | 2.03 | 1.94 | 1.84 | 1.73 | 1.60     |  |
| 120                                | 6.85                             | 4.79 | 3.95 | 3.48 | 3.17 | 2.96 | 2.79 | 2.66 | 2.56 | 2.47 | 2.34 | 2.19 | 2.03 | 1.95 | 1.86 | 1.76 | 1.66 | 1.53 | 1.38     |  |
| $\infty$                           | 6.63                             | 4.61 | 3.78 | 3.32 | 3.02 | 2.80 | 2.64 | 2.51 | 2.41 | 2.32 | 2.18 | 2.04 | 1.88 | 1.79 | 1.70 | 1.59 | 1.47 | 1.32 | 1.00     |  |

### 2.3.10 Curve Fitting

Very often in practice a relationship is found (or known) to exist between two or more variables. It is frequently desirable to express this relationship in mathematical form by determining an equation connecting the variables.

The first step is the collection of data showing corresponding values of the variables under consideration. From a scatter diagram, a plot of  $Y$  (ordinate) versus  $X$  (abscissa), it is often possible to visualize a smooth curve approximating the data. For purposes of reference, several types of approximating curves and their equations are listed. All letters other than  $X$  and  $Y$  represent constants.

- |                                                        |                             |
|--------------------------------------------------------|-----------------------------|
| 1. $Y = a_0 + a_1X$                                    | Straight line               |
| 2. $Y = a_0 + a_1X + a_2X^2$                           | Parabola or quadratic curve |
| 3. $Y = a_0 + a_1X + a_2X^2 + a_3X^3$                  | Cubic curve                 |
| 4. $Y = a_0 + a_1X + a_2 + \cdot \cdot \cdot + a_nX^n$ | $n$ th degree curve         |

As other possible equations (among many) used in practice, these may be mentioned:

- |                                                  |                            |
|--------------------------------------------------|----------------------------|
| 5. $Y = (a_0 + a_1X)^{-1}$ or $1/Y = a_0 + a_1X$ | Hyperbola                  |
| 6. $Y = ab^X$ or $\log Y = \log a + (\log b)_X$  | Exponential curve          |
| 7. $Y = aX^b$ or $\log Y = \log a + b \log X$    | Geometric curve            |
| 8. $Y = ab^X + g$                                | Modified exponential curve |
| 9. $Y = aX^n + g$                                | Modified geometric curve   |

When we draw a scatter plot of all  $X$  versus  $Y$  data, we see that some sort of shape can be described by the data points. From the scatter plot we can take a basic guess as to which type of curve will best describe the  $X$ — $Y$  relationship. To aid in the decision process, it is helpful to obtain scatter plots of transformed variables. For example, if a scatter plot of  $\log Y$  versus  $X$  shows a linear relationship, the equation has the form of number 6 above, while if  $\log Y$  versus  $\log X$  shows a linear relationship, the equation has the form of number 7. To facilitate this we frequently employ special graph paper for which one or both scales are calibrated logarithmically. These are referred to as *semilog* or *log-log graph paper*, respectively.

**2.3.10.1 The Least Squares or Best-fit Line.** The simplest type of approximating curve is a straight line, the equation of which can be written as in form number 1 above. It is customary to employ the above definition when  $X$  is the independent variable and  $Y$  is the dependent variable.

To avoid individual judgment in constructing any approximating curve to fit sets of data, it is necessary to agree on a definition of a *best-fit line*. One could construct what would be considered the best-fit line through the plotted pairs of data points. For a given value of  $X_1$ , there will be a difference  $D_1$  between the value  $Y_1$  and the constituent value  $\hat{Y}$  as determined by the calibration model. Since we are assuming that all the errors are in  $Y$ , we are seeking the best-fit line that minimizes the deviations in the  $Y$  direction between the experimental points and the calculated line. This condition will be met when the sum of squares for the differences, called residuals (or the sum of squares due to error),

$$\sum_{i=1}^N (Y_i - \hat{Y}_i)^2 \equiv \sum (D_1^2 + D_2^2 + \cdots + D_N^2)$$

is the least possible value when compared to all other possible lines fitted to that data. If the sum of squares for residuals is equal to zero, the calibration line is a perfect fit to the data. With a

mathematical treatment known as linear regression, one can find the “best” straight line through these real world points by minimizing the residuals.

This calibration model for the best-fit fit line requires that the line pass through the “centroid” of the points  $(\bar{X}, \bar{Y})$ . It can be shown that:

$$b = \frac{\sum_i (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_i (X_i - \bar{X})^2} \tag{2.17}$$

$$a = \bar{Y} - b\bar{X} \tag{2.18}$$

The line thus calculated is known as the line of regression of  $Y$  on  $X$ , that is, the line indicating how  $Y$  varies when  $X$  is set to chosen values.

If  $X$  is the dependent variable, the definition is modified by considering horizontal instead of vertical deviations. In general these two definitions lead to different least square curves.

*Example 13* The following data were recorded for the potential  $E$  of an electrode, measured against the saturated calomel electrode, as a function of concentration  $C$  (moles liter<sup>-1</sup>).

| $-\log C$ | $E, \text{ mV}$ | $-\log C$ | $E, \text{ mV}$ |
|-----------|-----------------|-----------|-----------------|
| 1.00      | 106             | 2.10      | 174             |
| 1.10      | 115             | 2.20      | 182             |
| 1.20      | 121             | 2.40      | 187             |
| 1.50      | 139             | 2.70      | 211             |
| 1.70      | 153             | 2.90      | 220             |
| 1.90      | 158             | 3.00      | 226             |

Fit the best straight line to these data;  $X_i$  represents  $-\log C$ , and  $Y_i$  represents  $E$ . We will perform the calculation manually, using the following tabular lay-out.

| $X_i$             | $Y_i$             | $(X_i - \bar{X})$ | $(X_i - \bar{X})^2$ | $(Y_i - \bar{Y})$ | $(X_i - \bar{X})(Y_i - \bar{Y})$ |
|-------------------|-------------------|-------------------|---------------------|-------------------|----------------------------------|
| 1.00              | 106               | -0.975            | 0.951               | -60               | 58.5                             |
| 1.10              | 115               | -0.875            | 0.766               | -51               | 44.6                             |
| 1.20              | 121               | -0.775            | 0.600               | -45               | 34.9                             |
| 1.50              | 139               | -0.475            | 0.226               | -27               | 12.8                             |
| 1.70              | 153               | -0.275            | 0.076               | -13               | 3.6                              |
| 1.90              | 158               | -0.075            | 0.006               | -8                | 0.6                              |
| 2.10              | 174               | +0.125            | 0.016               | 8                 | 1.0                              |
| 2.20              | 182               | 0.225             | 0.051               | 16                | 3.6                              |
| 2.40              | 187               | 0.425             | 0.181               | 21                | 8.9                              |
| 2.70              | 211               | 0.725             | 0.526               | 45                | 32.6                             |
| 2.90              | 220               | 0.925             | 0.856               | 54                | 50.0                             |
| 3.00              | 226               | 1.025             | 1.051               | 60                | 61.5                             |
| $\Sigma X_i$ 23.7 | $\Sigma Y_i$ 1992 | $\Sigma 0$        | $\Sigma 5.306$      | $\Sigma 0$        | $\Sigma 312.6$                   |
| $\bar{X} = 1.975$ | $\bar{Y} = 166$   |                   |                     |                   |                                  |

Now substituting the proper terms into Equation 17, the slope is:

$$b = \frac{312.6}{5.306} = 58.91$$

and from Equation 18, and substituting the “centroid” values of the points  $(\bar{X}, \bar{Y})$ , the intercept is:

$$a = 166 - 58.91(1.975) = 49.64$$

The best-fit equation is therefore:

$$E = 49.64 - 58.91 \log C$$

**2.3.10.2 Errors in the Slope and Intercept of the Best-fit Line.** Upon examination of the plot of pairs of data points, the calibration line, it will be obvious that the precision involved in analyzing an unknown sample will be considerably poorer than that indicated by replicate error alone. The scatter of these original points about the calibration line is a good measure of the error to be expected in analyzing an unknown sample. And this same error is considerably larger than the replication error because it will include other sources of variability due to a variety of causes. One possible source of variability might be the presence of different amounts of an extraneous material in the various samples used to establish the calibration curve. While this variability causes scatter about the calibration curve, it will not be reflected in the replication error of any one sample if the sample is homogeneous.

The scatter of the points around the calibration line or random errors are of importance since the best-fit line will be used to estimate the concentration of test samples by interpolation. The method used to calculate the random errors in the values for the slope and intercept is now considered. We must first calculate the standard deviation  $s_{Y/X}$ , which is given by:

$$s_{Y/X} = \sqrt{\frac{\sum_i (Y_i - \hat{Y})^2}{N - 2}} \quad (2.19)$$

Equation 19 utilizes the *Y-residuals*,  $Y_i - \hat{Y}$ , where  $\hat{Y}_i$  are the points on the calculated best-fit line or the fitted  $Y_i$  values. The appropriate number of degrees of freedom is  $N - 2$ ; the minus 2 arises from the fact that linear calibration lines are derived from both a slope and an intercept which leads to a loss of two degrees of freedom.

Now we can calculate the standard deviations for the slope and the intercept. These are given by:

$$s_b = \frac{s_{Y/X}}{\sqrt{\sum_i (X_i - \bar{X})^2}} \quad (2.20)$$

$$s_a = s_{Y/X} \sqrt{\frac{\sum_i X_i^2}{N \sum_i (X_i - \bar{X})^2}} \quad (2.21)$$

The confidence limits for the slope are given by  $b \pm t_b$ , where the  $t$ -value is taken at the desired confidence level and  $(N - 2)$  degrees of freedom. Similarly, the confidence limits for the intercept are given by  $a \pm ts_a$ . The closeness of  $\hat{x}$  to  $x_i$  is answered in terms of a confidence interval for  $x_0$  that extends from an upper confidence (UCL) to a lower confidence (LCL) level. Let us choose 95% for the confidence interval. Then, remembering that this is a two-tailed test (UCL and LCL), we obtain from a table of Student's  $t$  distribution the critical value of  $t_c$  ( $t_{0.975}$ ) and the appropriate number of degrees of freedom.

*Example 14* For the best-fit line found in Example 13, express the result in terms of confidence intervals for the slope and intercept. We will choose 95% for the confidence interval.

The standard deviation  $s_{Y/X}$  is given by Equation 19, but first a supplementary table must be constructed for the  $Y$  residuals and other data which will be needed in subsequent equations.

| $\hat{Y}$      | $(Y_i - \hat{Y})$ | $(Y_i - \hat{Y})^2$ | $X_i^2$ |
|----------------|-------------------|---------------------|---------|
| 108.6          | 2.55              | 6.50                | 1.00    |
| 114.4          | -0.56             | 0.31                | 1.21    |
| 120.3          | -0.67             | 0.45                | 1.44    |
| 138.0          | -1.00             | 1.00                | 2.25    |
| 149.8          | -3.21             | 10.32               | 2.89    |
| 161.6          | 3.57              | 12.94               | 3.61    |
| 173.4          | -0.65             | 0.42                | 4.41    |
| 179.2          | -2.76             | 7.61                | 4.84    |
| 191.0          | 4.02              | 16.16               | 5.76    |
| 208.7          | -2.30             | 5.30                | 7.29    |
| 220.5          | 0.48              | 0.23                | 8.41    |
| 226.4          | 0.40              | 0.16                | 9.00    |
| $\Sigma$ 61.20 |                   | $\Sigma$ 52.11      |         |

Now substitute the appropriate values into Equation 19 where there are  $12 - 2 = 10$  degrees of freedom:

$$s_{X/Y} = \sqrt{\frac{61.20}{10}} = 2.47$$

We can now calculate  $s_b$  and  $s_a$  from Equations 20 and 21, respectively:

$$s_b = \frac{s_{Y/X}}{\sqrt{5.31}} = 1.07$$

and

$$s_a = 2.47 \sqrt{\frac{52.11}{12(5.306)}} = 2.23$$

Now, using a two-tailed value for Student's  $t$ :

$$b \pm ts_b = 58.91 \pm 2.23(1.07) = 58.91 \pm 2.39$$

$$a \pm ts_a = 49.64 \pm 2.23(2.23) = 49.64 \pm 4.97$$



The best-fit equation expressed in terms of the confidence intervals for the slope and intercept is:

$$E = (49.6_4 \pm 5.0) - (58.9_1 \pm 2.43) \log C$$

To conclude the discussion about the best-fit line, the following relationship can be shown to exist among  $Y$ ,  $\hat{Y}$ , and  $\bar{Y}$ :

$$\sum_{i=1}^N (Y_i - \bar{Y})^2 = \sum_{i=1}^N (\hat{Y}_i - \bar{Y})^2 + \sum_{i=1}^N (Y_i - \hat{Y}_i)^2 \quad (2.22)$$

The term on the left-hand side is a constant and depends only on the constituent values provided by the reference laboratory and does not depend in any way upon the calibration. The two terms on the right-hand side of the equation show how this constant value is apportioned between the two quantities that are themselves summations, and are referred to as the sum of squares due to regression and the sum of squares due to error. The latter will be the smallest possible value that it can possibly be for the given data.

### 2.3.11 Control Charts

It is often important in practice to know when a process has changed sufficiently so that steps may be taken to remedy the situation. Such problems arise in quality control where one must, often quickly, decide whether observed changes are due to simple chance fluctuations or to actual changes in the amount of a constituent in successive production lots, mistakes of employees, etc. Control charts provide a useful and simple method for dealing with such problems.

The chart consists of a central line and two pairs of limit lines or simply of a central line and one pair of control limits. By plotting a sequence of points in order, a continuous record of the quality characteristic is made available. Trends in data or sudden lack of precision can be made evident so that the causes may be sought.

The control chart is set up to answer the question of whether the data are in statistical control, that is, whether the data may be regarded as random samples from a single population of data. Because of this feature of testing for randomness, the control chart may be useful in searching out systematic sources of error in laboratory research data as well as in evaluating plant-production or control-analysis data.<sup>1</sup>

To set up a control chart, individual observations might be plotted in sequential order and then compared with control limits established from sufficient past experience. Limits of  $\pm 1.96\sigma$  corresponding to a confidence level of 95%, might be set for control limits. The probability of a future observation falling outside these limits, based on chance, is only 1 in 20. A greater proportion of scatter might indicate a nonrandom distribution (a systematic error). It is common practice with some users of control charts to set inner control limits, or warning limits, at  $\pm 1.96\sigma$  and outer control limits of  $\pm 3.00\sigma$ . The outer control limits correspond to a confidence level of 99.8%, or a probability of 0.002 that a point will fall outside the limits. One-half of this probability corresponds to a high result and one-half to a low result. However, other confidence limits can be used as well; the choice in each case depends on particular circumstances.

Special attention should be paid to one-sided deviation from the control limits, because systematic errors more often cause deviation in one direction than abnormally wide scatter. Two systematic errors of opposite sign would of course cause scatter, but it is unlikely that both would have entered at the same time. It is not necessary that the control chart be plotted in a time sequence. In any

<sup>1</sup> G. Wernimont, *Ind. Eng. Chem., Anal. Ed.* **18**:587 (1946); J. A. Mitchell, *ibid.* **19**:961 (1947).

situation where relatively large numbers of units or small groups are to be compared, the control chart is a simple means of indicating whether any unit or group is out of line. Thus laboratories, production machines, test methods, or analysts may be put arbitrarily into a horizontal sequence.

Usually it is better to plot the means of small groups of observations on a control chart, rather than individual observations. The random scatter of averages of pairs of observations is  $1/(2)^{1/2} = 0.71$  as great as that of single observations, and the likelihood of two “wild” observations in the same direction is vanishing small. The groups of two to five observations should be chosen in such a way that only change variations operate within the group, whereas assignable causes are sought for variations between groups. If duplicate analyses are performed each day, the pairs form logical groups.

Some measure of dispersion of the subgroup data should also be plotted as a parallel control chart. The most reliable measure of scatter is the standard deviation. For small groups, the range becomes increasingly significant as a measure of scatter, and it is usually a simple matter to plot the range as a vertical line and the mean as a point on this line for each group of observations.

## Bibliography

- Alder, H. L., and E. B. Roessler, *Introduction to Probability and Statistics*, W. H. Freeman, San Francisco, 1972.
- Bergmann, B., B. von Oepen, and P. Zinn, *Anal. Chem.*, **59**:2532 (1987).
- Box, G., W. Hunter, and J. Hunter, *Statistics for Experimenters*, Wiley, New York, 1978.
- Clayton, C. A., J. W. Hines, and P. D. Elkins, *Anal. Chem.*, **59**:2506 (1987).
- Caulcutt, R., and R. Boddy, *Statistics for Analytical Chemists*, Chapman and Hall, London, 1983.
- Dixon, W. J., and F. J. Massey, *Introduction to Statistical Analysis*, McGraw-Hill, New York, 1969.
- Hirsch, R. F. “Analysis of Variance in Analytical Chemistry,” *Anal. Chem.*, **49**:691A (1977).
- Jaffe, A. J., and H. F. Spirer, *Misused Statistics—Straight Talk for Twisted Numbers*, Marcel Dekker, New York, 1987.
- Linnig, F. J., and J. Mandel, “Which Measure of Precision?” *Anal. Chem.*, **36**:25A (1964).
- Mark, H., and J. Workman, *Statistics in Spectroscopy*, Academic Press, San Diego, CA, 1991.
- Meier, P. C., and R. E. Zund, *Statistical Methods in Analytical Chemistry*, Wiley, New York, 1993.
- Miller, J. C., and J. N. Miller, *Statistics for Analytical Chemists*, Halsted Press, John Wiley, New York, 1984.
- Moore, D. S., *Statistics: Concepts and Controversies*, W. H. Freeman, New York, 1985.
- Mulholland, H., and C. R. Jones, *Fundamentals of Statistics*, Plenum Press, New York, 1968.
- Taylor, J. K., *Statistical Techniques for Data Analysis*, Lewis, Boca Raton, FL, 1990.
- Youden, W. J., “The Sample, the Procedure, and the Laboratory,” *Anal. Chem.*, **32**:23A (1960).
- Youden, W. J., *Statistical Methods for Chemists*, Wiley, New York, 1951.
- Youden, W. J., *Statistical Manual of the AOAC*, AOAC, 1111 North 19th St., Arlington, VA, 22209.

---

# SECTION 3

---

## INORGANIC CHEMISTRY

---

|                                                            |             |
|------------------------------------------------------------|-------------|
| <b>3.1 NOMENCLATURE OF INORGANIC COMPOUNDS</b>             | <b>3.1</b>  |
| <b>3.1.1 Writing Formulas</b>                              | <b>3.1</b>  |
| <b>3.1.2 Naming Compounds</b>                              | <b>3.3</b>  |
| <b>3.1.3 Cations</b>                                       | <b>3.6</b>  |
| <b>3.1.4 Anions</b>                                        | <b>3.6</b>  |
| <b>3.1.5 Acids</b>                                         | <b>3.8</b>  |
| <b>3.1.6 Salts and Functional Derivatives of Acids</b>     | <b>3.8</b>  |
| <b>Table 3.1 Trivial Names Retained for Acids</b>          | <b>3.9</b>  |
| <b>3.1.7 Coordination Compounds</b>                        | <b>3.10</b> |
| <b>3.1.8 Addition Compounds</b>                            | <b>3.11</b> |
| <b>3.2 PHYSICAL PROPERTIES OF PURE SUBSTANCES</b>          | <b>3.12</b> |
| <b>Table 3.2 Physical Constants of Inorganic Compounds</b> | <b>3.12</b> |
| <b>Table 3.3 Synonyms and Mineral Names</b>                | <b>3.61</b> |

---

### 3.1 NOMENCLATURE OF INORGANIC COMPOUNDS

---

The following synopsis of rules for naming inorganic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see G. J. Leigh (ed.), *Nomenclature of Inorganic Chemistry*, 3d ed., Blackwell Scientific Publications, Oxford, 1990. This 289-page publication contains the Recommendations 1990 of the Commission on Nomenclature of Inorganic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC). In particular, the latest report should be consulted for coordination compounds, boron compounds, and crystalline phases of variable composition.

#### 3.1.1 Writing Formulas

**3.1.1.1 Mass Number, Atomic Number, Number of Atoms, and Ionic Charge.** The mass number, atomic number, number of atoms, and ionic charge of an element are indicated by means of four indices placed around the symbol:

|               |               |                 |                     |
|---------------|---------------|-----------------|---------------------|
| mass number   | <b>SYMBOL</b> | ionic charge    | $^{15}\text{N}_2^-$ |
| atomic number |               | number of atoms |                     |

Ionic charge should be indicated by an Arabic superscript numeral preceding the plus or minus sign:  $\text{Mg}^{2+}$ ,  $\text{PO}_4^{3-}$ .

**3.1.1.2 Placement of Atoms in a Formula.** The electropositive constituent (cation) is placed first in a formula. If the compound contains more than one electropositive or more than one electronegative constituent, the sequence within each class should be in alphabetical order of their symbols.

The alphabetical order may be different in formulas and names; for example,  $\text{NaNH}_4\text{HPO}_4$ , ammonium sodium hydrogen phosphate.

Acids are treated as hydrogen salts. Hydrogen is cited last among the cations.

When there are several types of ligands, anionic ligands are cited before the neutral ligands.

**3.1.1.3 Binary Compounds between Nonmetals.** For binary compounds between nonmetals, that constituent should be placed first which appears earlier in the sequence:

Rn, Xe, Kr, Ar, Ne, He, B, Si, C, Sb, As, P, N, H, Te, Se, S, At, I, Br, Cl, O, F

*Examples:*  $\text{AsCl}_3$ ,  $\text{SbH}_3$ ,  $\text{H}_3\text{Te}$ ,  $\text{BrF}_3$ ,  $\text{OF}_2$ , and  $\text{N}_4\text{S}_4$ .

**3.1.1.4 Chain Compounds.** For chain compounds containing three or more elements, the sequence should be in accordance with the order in which the atoms are actually bound in the molecule or ion.

*Examples:*  $\text{SCN}^-$  (thiocyanate),  $\text{HSCN}$  (hydrogen thiocyanate or thiocyanic acid),  $\text{HNCO}$  (hydrogen isocyanate),  $\text{HONC}$  (hydrogen fulminate), and  $\text{HPH}_2\text{O}_2$  (hydrogen phosphinate).

**3.1.1.5 Use of Centered Period.** A centered period is used to denote water of hydration, other solvates, and addition compounds; for example,  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ , copper(II) sulfate 5-water (or pentahydrate).

**3.1.1.6 Free Radicals.** In the formula of a polyatomic radical an unpaired electron(s) is(are) indicated by a dot placed as a right superscript to the parentheses (or square bracket for coordination compounds). In radical ions the dot precedes the charge. In structural formulas, the dot may be placed to indicate the location of the unpaired electron(s).

*Examples:*  $(\text{HO})^\cdot$   $(\text{O}_2)^{2\cdot}$   $(\dot{\text{N}}\text{H}_3)$

**3.1.1.7 Enclosing Marks.** Where it is necessary in an inorganic formula, enclosing marks (parentheses, braces, and brackets) are nested within square brackets as follows:

$[()]$ ,  $[{} \{ () \}]$ ,  $[{} \{ [ () ] \}]$ ,  $[{} \{ [ {} \{ () \} ] \}]$

In an inorganic name the nesting order is different:  $\{ \{ \{ [ () ] \} \} \}$ , and so on.

**3.1.1.8 Molecular Formula.** For compounds consisting of discrete molecules, a formula in accordance with the correct molecular weight of the compound should be used.

*Examples:*  $\text{S}_2\text{Cl}_2$ ,  $\text{S}_8$ ,  $\text{N}_2\text{O}_4$ , and  $\text{H}_4\text{P}_2\text{O}_6$ ; not  $\text{SCl}$ ,  $\text{S}$ ,  $\text{NO}_2$ , and  $\text{H}_2\text{PO}_3$ .

**3.1.1.9 Structural Formula and Prefixes.** In the structural formula the sequence and spatial arrangement of the atoms in a molecule are indicated.

*Examples:*  $\text{NaO}(\text{O}=\text{C})\text{H}$  (sodium formate),  $\text{Cl}-\text{S}-\text{S}-\text{Cl}$  (disulfur dichloride).

Structural prefixes should be italicized and connected with the chemical formula by a hyphen: *cis-*, *trans-*, *anti-*, *syn-*, *cyclo-*, *catena-*, *o-* or *ortho-*, *m-* or *meta-*, *p-* or *para-*, *sec-* (secondary), *tert-* (tertiary), *v-* (vicinal), *meso-*, *as-* for asymmetrical, and *s-* for symmetrical.

The sign of optical rotation is placed in parentheses, (+) for dextrorotary, (−) for levorotary, and (±) for racemic, and placed before the formula. The wavelength (in nanometers) is indicated by a right subscript; unless indicated otherwise, it refers to the sodium D-line.

The italicized symbols *d*- (for deuterium) and *t*- (for tritium) are placed after the formula and connected to it by a hyphen. The number of deuterium or tritium atoms is indicated by a subscript to the symbol.

*Examples:*

|                                                                  |                                                          |
|------------------------------------------------------------------|----------------------------------------------------------|
| <i>cis</i> -[PtCl <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> ] | methan- <i>d</i> <sub>3</sub> -ol                        |
| di- <i>tert</i> -butyl sulfate                                   | (+) <sub>589</sub> [Co(en) <sub>3</sub> ]Cl <sub>2</sub> |
| methan-ol- <i>d</i>                                              |                                                          |

### 3.1.2 Naming Compounds

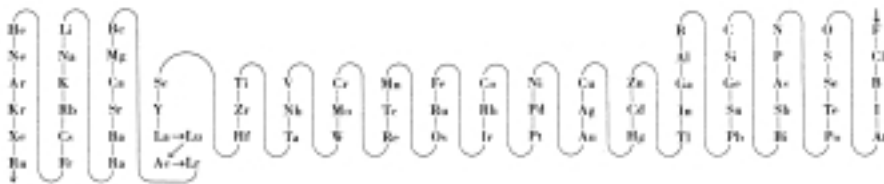
**3.1.2.1 Names and Symbols for Elements.** Names and symbols for the elements are given in Table 3.2. Wolfram is preferred to tungsten but the latter is used in the United States. In forming a complete name of a compound, the name of the electropositive constituent is left unmodified except when it is necessary to indicate the valency (see oxidation number and charge number, formerly the Stock and Ewens-Bassett systems). The order of citation follows the alphabetical listing of the names of the cations followed by the alphabetical listing of the anions and ligands. The alphabetical citation is maintained regardless of the number of each ligand.

*Example:* K[AuS(S<sub>2</sub>)] is potassium (disulfido)thioaurate(1-).

**3.1.2.2 Electronegative Constituents.** The name of a monatomic electronegative constituent is obtained from the element name with its ending (-en, -ese, -ic, -ine, -ium, -ogen, -on, -orus, -um, -ur, -y, or -ygen) replaced by -ide. The elements bismuth, cobalt, nickel, zinc, and the noble gases are used unchanged with the ending -ide. Homopolyatomic ligands will carry the appropriate prefix. A few Latin names are used with affixes: cupr- (copper), aur- (gold), ferr- (iron), plumb- (lead), argent- (silver), and stann- (tin).

For binary compounds the name of the element standing later in the sequence in Sec. 3.1.1.3 is modified to end in -ide. Elements other than those in the sequence of Sec. 3.1.1.3 are taken in the reverse order of the following sequence, and the name of the element occurring last is modified to end in -ide; e.g., calcium stannide.

#### ELEMENT SEQUENCE



**3.1.2.3 Stoichiometric Proportions.** The stoichiometric proportions of the constituents in a formula may be denoted by Greek numerical prefixes: mono-, di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona- (Latin), deca-, undeca- (Latin), dodeca-, . . . , icos- (20), henicos- (21), . . . , triconta- (30), tetraconta- (40), . . . , hecta- (100), and so on, preceding without a hyphen the names of the elements to which they refer. The prefix mono can usually be omitted; occasionally hemi- (½) and sesqui- (¾) are used. No elisions are made when using numerical prefixes except in the case of icos- when the letter “i” is elided in docosa- and tricos-. Beyond 10, prefixes may be replaced by Arabic numerals.

When it is required to indicate the number of entire groups of atoms, the multiplicative numerals bis-, tris-, tetrakis-, pentakis-, and so on, are used (i.e., -kis is added starting from tetra-). The entity to which they refer is placed in parentheses.

*Examples:*  $\text{Ca}[\text{PF}_6]_2$ , calcium bis(hexafluorophosphate); and  $(\text{C}_{10}\text{H}_{21})_3\text{PO}_4$ , tris(decyl) phosphate instead of tridecyl which is  $(\text{C}_{13}\text{H}_{27}-)$ .

Composite numeral prefixes are built up by citing units first, then tens, then hundreds, and so on. For example, 43 is written tritetraconta- (or tritetracontakis-).

In indexing it may be convenient to italicize a numerical prefix at the beginning of the name and connect it to the rest of the name with a hyphen; e.g., *di*-nitrogen pentaoxide (indexed under the letter “n”).

**3.1.2.4 Oxidation and Charge Numbers.** The *oxidation number* (Stock system) of an element is indicated by a Roman numeral placed in parentheses immediately following the name of the element. For zero, the cipher 0 is used. When used in conjunction with symbols the Roman numeral may be placed above and to the right. The *charge number* of an ion (Ewens-Bassett system) rather than the oxidation state is indicated by an Arabic numeral followed by the sign of the charge cited and is placed in parentheses immediately following the name of the ion.

*Examples:*  $\text{P}_2\text{O}_5$ , diphosphorus pentaoxide or phosphorus(V) oxide;  $\text{Hg}_2^{2+}$ , mercury(I) ion or dimercury(2+) ion;  $\text{K}_2[\text{Fe}(\text{CN})_6]$ , potassium hexacyanoferrate(II) or potassium hexacyanoferrate(4-);  $\text{Pb}_2^{\text{II}}\text{Pb}^{\text{IV}}\text{O}_4$ , dilead(II) lead(IV) oxide or trilead tetraoxide.

Where it is not feasible to define an oxidation state for each individual member of a group, the overall oxidation level of the group is defined by a formal ionic charge to avoid the use of fractional oxidation states; for example,  $\text{O}_2^-$ .

**3.1.2.5 Collective Names.** Collective names include:

Halogens (F, Cl, Br, I, At)

Chalcogens (O, S, Se, Te, Po)

Alkali metals (Li, Na, K, Rb, Cs, Fr)

Alkaline-earth metals (Ca, Sr, Ba, Ra)

Lanthanoids or lanthanides (La to Lu)

Rare-earth metals (Sc, Y, and La to Lu inclusive)

Actinoids or actinides (Ac to Lr, those whose 5f shell is being filled)

Noble gases (He to Rn)

A transition element is an element whose atom has an incomplete *d* subshell, or which gives rise to a cation or cations with an incomplete *d* subshell.

**3.1.2.6 Isotopically Labeled Compounds.** The hydrogen isotopes are given special names:  $^1\text{H}$  (protium),  $^2\text{H}$  or D (deuterium), and  $^3\text{H}$  or T (tritium). The superscript designation is preferred because D and T disturb the alphabetical ordering in formulas.

Other isotopes are designated by mass numbers:  $^{10}\text{B}$  (boron-10).

Isotopically labeled compounds may be described by inserting the italic symbol of the isotope in brackets into the name of the compound; for example,  $\text{H}^{36}\text{Cl}$  is hydrogen chloride[ $^{36}\text{Cl}$ ] or hydrogen chloride-36, and  $^2\text{H}^{38}\text{Cl}$  is hydrogen [ $^2\text{H}$ ] chloride[ $^{38}\text{Cl}$ ] or hydrogen-2 chloride-38.

**3.1.2.7 Allotropes.** Systematic names for gaseous and liquid modifications of elements are sometimes needed. Allotropic modifications of an element bear the name of the atom together with the descriptor to specify the modification. The following are a few common examples:

| Symbol         | Trivial name                      | Systematic name |
|----------------|-----------------------------------|-----------------|
| H              | Atomic hydrogen                   | Monohydrogen    |
| O <sub>2</sub> | (Common oxygen)                   | Dioxygen        |
| O <sub>3</sub> | Ozone                             | Trixygen        |
| P <sub>4</sub> | White phosphorus                  | Tetraphosphorus |
| S <sub>8</sub> | $\alpha$ -Sulfur, $\beta$ -Sulfur | Octasulfur      |
| S <sub>n</sub> | $\mu$ -Sulfur (plastic sulfur)    | Polysulfur      |

Trivial (customary) names are used for the amorphous modification of an element.

**3.1.2.8 Heteroatomic and Other Anions.** A few heteroatomic anions have names ending in -ide. These are

|                                                         |                                         |
|---------------------------------------------------------|-----------------------------------------|
| —OH, hydroxide ion (not hydroxyl)                       | —NH—, imide ion                         |
| —CN, cyanide ion                                        | —NH—NH <sub>2</sub> , hydrazide ion     |
| —HF <sub>2</sub> <sup>−</sup> , hydrogen difluoride ion | —NHOH, hydroxylamide ion                |
| —NH <sub>2</sub> , amide ion                            | —HS <sup>−</sup> , hydrogen sulfide ion |

Added to these anions are

|                                              |                      |
|----------------------------------------------|----------------------|
| —I <sub>3</sub> <sup>−</sup> , triiodide ion | —O—O—, peroxide ion  |
| —N <sub>3</sub> , azide ion                  | —S—S—, disulfide ion |
| —O <sub>3</sub> , ozonide ion                |                      |

**3.1.2.9 Binary Compounds of Hydrogen.** Binary compounds of hydrogen with the more electropositive elements are designated hydrides (NaH, sodium hydride).

Volatile hydrides, except those of Periodic Group VII and of oxygen and nitrogen, are named by citing the root name of the element (penultimate consonant and Latin affixes, Sec. 3.1.2.2) followed by the suffix -ane. Exceptions are water, ammonia, hydrazine, phosphine, arsine, stibine, and bismuthine.

*Examples:* B<sub>2</sub>H<sub>6</sub>, diborane; B<sub>10</sub>H<sub>14</sub>, decaborane(14); B<sub>10</sub>H<sub>16</sub>, decaborane(16); P<sub>2</sub>H<sub>4</sub>, diphosphane; Sn<sub>2</sub>H<sub>6</sub>, distannane; H<sub>2</sub>Se<sub>2</sub>, diselane; H<sub>2</sub>Te<sub>2</sub>, ditellane; H<sub>2</sub>S<sub>5</sub>, pentasulfane; and PbH<sub>4</sub>, plum-bane.

**3.1.2.10 Neutral Radicals.** Certain neutral radicals have special names ending in -yl:

|                  |            |                  |                  |
|------------------|------------|------------------|------------------|
| HO               | hydroxyl   | ClO <sub>3</sub> | perchloryl*      |
| CO               | carbonyl   | CrO <sub>2</sub> | chromyl          |
| ClO              | chlorosyl* | NO               | nitrosyl         |
| ClO <sub>2</sub> | chloryl*   | NO <sub>2</sub>  | nitryl (nitroyl) |

\* Similarly for the other halogens.

|                               |                     |                  |           |
|-------------------------------|---------------------|------------------|-----------|
| PO                            | phosphoryl          | SeO              | seleninyl |
| SO                            | sulfinyl (thionyl)  | SeO <sub>2</sub> | selenonyl |
| SO <sub>2</sub>               | sulfonyl (sulfuryl) | UO <sub>2</sub>  | uranyl    |
| S <sub>2</sub> O <sub>5</sub> | disulfuryl          | NpO <sub>2</sub> | neptunyl† |

Radicals analogous to the above containing other chalcogens in place of oxygen are named by adding the prefixes thio-, seleno-, and so on; for example, PS, thiophosphoryl; CS, thiocarbonyl.

### 3.1.3 Cations

**3.1.3.1 Monatomic Cations.** Monatomic cations are named as the corresponding element; for example, Fe<sup>2+</sup>, iron(II) ion; Fe<sup>3+</sup>, iron(III) ion.

This principle also applies to polyatomic cations corresponding to radicals with special names ending in -yl (Sec. 3.1.2.10); for example, PO<sup>+</sup>, phosphoryl cation; NO<sup>+</sup>, nitrosyl cation; NO<sub>2</sub><sup>+</sup>, nitryl cation; O<sub>2</sub><sup>+</sup>, oxygenyl cation.

Use of the oxidation number and charge number extends the range for radicals; for example, UO<sub>2</sub><sup>+</sup> uranyl(VI) or uranyl(2+) cation; UO<sub>2</sub><sup>+</sup>, uranyl(V) or uranyl(1+) cation.

**3.1.3.2 Polyatomic Cations.** Polyatomic cations derived by addition of more protons than required to give a neutral unit to polyatomic anions are named by adding the ending -onium to the root of the name of the anion element; for example, PH<sub>4</sub><sup>+</sup>, phosphonium ion; H<sub>2</sub>I<sup>+</sup>, iodonium ion; H<sub>3</sub>O<sup>+</sup>, oxonium ion; CH<sub>3</sub>OH<sub>2</sub><sup>+</sup>, methyl oxonium ion.

*Exception:* The name ammonium is retained for the NH<sub>4</sub><sup>+</sup> ion; similarly for substituted ammonium ions; for example, NF<sub>4</sub><sup>+</sup>, tetrafluoroammonium ion.

Substituted ammonium ions derived from nitrogen bases with names ending in -amine receive names formed by changing -amine into -ammonium. When known by a name not ending in -amine, the cation name is formed by adding the ending -ium to the name of the base (eliding the final vowel); e.g., anilinium, hydrazinium, imidazolium, acetonium, dioxanium.

Exceptions are the names uronium and thiouronium derived from urea and thiourea, respectively.

**3.1.3.3 Multiple Ions from One Base.** Where more than one ion is derived from one base, the ionic charges are indicated in their names: N<sub>2</sub>H<sub>5</sub><sup>+</sup>, hydrazinium(1+) ion; N<sub>2</sub>H<sub>6</sub><sup>2+</sup>, hydrazinium(2+) ion.

### 3.1.4 Anions

See Secs. 3.1.2.2 and 3.1.2.8 for naming monatomic and certain polyatomic anions. When an organic group occurs in an inorganic compound, organic nomenclature (*q.v.*) is followed to name the organic part.

**3.1.4.1 Protonated Anions.** Ions such as HSO<sub>4</sub><sup>-</sup> are recommended to be named hydrogensulfate with the two words written as one following the usual practice for polyatomic anions. However, in the *Nomenclature of Organic Chemistry*, 1979 edition, hydrogen is used as a separate word; this practice is followed in this Handbook.

† Similarly for the other actinoid elements.



**3.1.4.2 Other Polyatomic Anions.** Names for other polyatomic anions consist of the root name of the central atom with the ending -ate and followed by the valence of the central atom expressed by its oxidation number. Atoms and groups attached to the central atom are treated as ligands in a complex.

*Examples:*  $[\text{Sb}(\text{OH})_6]^-$ , hexahydroxoantimonate(V);  $[\text{Fe}(\text{CN})_6]^{3-}$ , hexacyanoferrate(III);  $[\text{Co}(\text{NO}_2)_6]^{3-}$ , hexanitritocobaltate(III);  $[\text{TiO}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]^{2-}$ , oxobisoxalatodiaquatitanate(IV);  $[\text{PCl}_6]^-$ , hexachlorophosphate(V).

Exceptions to the use of the root name of the central atom are antimonate, bismuthate, carbonate, cobaltate, nickelate (or niccolate), nitrate, phosphate, tungstate (or wolframate), and zincate.

**3.1.4.3 Anions of Oxygen.** Oxygen is treated in the same manner as other ligands with the number of -oxo groups indicated by a suffix; for example,  $\text{SO}_3^{2-}$ , trioxosulfate.

The ending -ite, formerly used to denote a lower state of oxidation, may be retained in trivial names in these cases (note Sec. 3.1.5.3 also):

|                             |              |                             |               |
|-----------------------------|--------------|-----------------------------|---------------|
| $\text{AsO}_3^{3-}$         | arsenite     | $\text{NOO}_2^-$            | peroxonitrite |
| $\text{BrO}^-$              | hypobromite  | $\text{PO}_3^{3-}$          | phosphite*    |
| $\text{ClO}^-$              | hypochlorite | $\text{SO}_3^{2-}$          | sulfite       |
| $\text{ClO}_2^-$            | chlorite     | $\text{S}_2\text{O}_5^{2-}$ | disulfite     |
| $\text{IO}^-$               | hypoiodite   | $\text{S}_2\text{O}_4^{2-}$ | dithionite    |
| $\text{NO}_2^-$             | nitrite      | $\text{S}_2\text{O}_3^{2-}$ | thiosulfite   |
| $\text{N}_2\text{O}_2^{2-}$ | hyponitrite  | $\text{SeO}_3^{2-}$         | selenite      |

However, compounds known to be double oxides in the solid state are named as such; for example,  $\text{Cr}_2\text{CuO}_4$  (actually  $\text{Cr}_2\text{O}_3 \cdot \text{CuO}$ ) is chromium(III) copper(II) oxide (and not copper chromite).

**3.1.4.4 Isopolyanions.** Isopolyanions are named by indicating with numerical prefixes the number of atoms of the characteristic element. It is not necessary to give the number of oxygen atoms when the charge of the anion or the number of cations is indicated.

*Examples:*  $\text{Ca}_3\text{Mo}_7\text{O}_{24}$ , tricalcium 24-oxoheptamolybdate, may be shortened to tricalcium heptamolybdate; the anion,  $\text{Mo}_7\text{O}_{24}^{6-}$ , is heptamolybdate(6-);  $\text{S}_2\text{O}_7^{2-}$ , disulfate(2-);  $\text{P}_2\text{O}_7^{4-}$ , diphosphate(V)(4-).

When the characteristic element is partially or wholly present in a lower oxidation state than corresponds to its Periodic Group number, oxidation numbers are used; for example,  $[\text{O}_2\text{HP}-\text{O}-\text{PO}_3\text{H}]^{2-}$ , dihydrogendiphosphate(III,V)(2-).

A bridging group should be indicated by adding the Greek letter  $\mu$  immediately before its names and separating this from the rest of the complex by a hyphen. The atom or atoms of the characteristic element to which the bridging atom is bonded, is indicated by numbers.

*Examples:*  $[\text{O}_3\text{P}-\text{S}-\text{PO}_2-\text{O}-\text{PO}_3]^{5-}$ , 1,2- $\mu$ -thiotriphosphate(5-)  
 $[\text{S}_3\text{P}-\text{O}-\text{PS}_2-\text{O}-\text{PS}_3]^{5-}$ , di- $\mu$ -oxo-octathiotriphosphate(5-)

\* Named for esters formed from the hypothetical acid  $\text{P}(\text{OH})_3$ .

### 3.1.5 Acids

**3.1.5.1 Acids and -ide Anions.** Acids giving rise to the -ide anions (Sec. 3.1.2.2) should be named as hydrogen . . . -ide; for example, HCl, hydrogen chloride;  $\text{HN}_3$ , hydrogen azide.

Names such as hydrobromic acid refer to an aqueous solution, and percentages such as 48% HBr denote the weight/volume of hydrogen bromide in the solution.

**3.1.5.2 Acids and -ate Anions.** Acids giving rise to anions bearing names ending in -ate are treated as in Sec. 3.1.5.1; for example,  $\text{H}_2\text{GeO}_4$ , hydrogen germanate;  $\text{H}_4[\text{Fe}(\text{CN})_6]$ , hydrogen hexacyanoferrate(II).

**3.1.5.3 Trivial Names.** Acids given in Table 3.1 retain their trivial names due to long-established usage. Anions may be formed from these trivial names by changing -ous acid to -ite, and -ic acid to -ate. The prefix hypo- is used to denote a lower oxidation state and the prefix per- designates a higher oxidation state. The prefixes ortho- and meta- distinguish acids of differing water content; for example,  $\text{H}_4\text{SiO}_4$  is orthosilicic acid and  $\text{H}_2\text{SiO}_3$  is metasilicic acid. The anions would be named silicate(4-) and silicate(2-), respectively.

**3.1.5.4 Peroxo- Group.** When used in conjunction with the trivial names of acids, the prefix peroxo- indicates substitution of  $\text{—O—}$  by  $\text{—O—O—}$ .

**3.1.5.5 Replacement of Oxygen by Other Chalcogens.** Acids derived from oxoacids by replacement of oxygen by sulfur are called thioacids, and the number of replacements are given by prefixes di-, tri-, and so on. The affixes seleno- and telluro- are used analogously.

*Examples:*  $\text{HOO—C=S}$ , thiocarbonic acid;  $\text{HSS—C=S}$ , trithiocarbonic acid.

**3.1.5.6 Ligands Other than Oxygen and Sulfur.** See Sec. 3.1.7, Coordination Compounds, for acids containing ligands other than oxygen and sulfur (selenium and tellurium).

**3.1.5.7 Differences between Organic and Inorganic Nomenclature.** Organic nomenclature is largely built upon the scheme of substitution, that is, the replacement of hydrogen atoms by other atoms or groups. Although rare in inorganic nomenclature:  $\text{NH}_2\text{Cl}$  is called chloramine and  $\text{NHCl}_2$  dichloroamine. Other substitutive names are fluorosulfonic acid and chlorosulfonic acid derived from  $\text{HSO}_3\text{H}$ . These and the names aminosulfonic acid (sulfamic acid), iminodisulfonic acid, and nitritrisulfonic acid should be replaced by the following based on the concept that these names are formed by adding hydroxyl, amide, imide, and so on, groups together with oxygen atoms to a sulfur atom:

|                                  |                     |                                    |                            |
|----------------------------------|---------------------|------------------------------------|----------------------------|
| $\text{HSO}_3\text{F}$           | fluorosulfuric acid | $\text{NH}(\text{SO}_3\text{H})_2$ | imidobis(sulfuric) acid    |
| $\text{HSO}_3\text{Cl}$          | chlorosulfuric acid | $\text{N}(\text{SO}_3\text{H})_3$  | nitridotris(sulfuric) acid |
| $\text{NH}_2\text{SO}_3\text{H}$ | amidosulfuric acid  |                                    |                            |

### 3.1.6 Salts and Functional Derivatives of Acids

**3.1.6.1 Acid Halogenides.** For acid halogenides the name is formed from the corresponding acid radical if this has a special name (Sec. 3.1.2.10); for example,  $\text{NOCl}$ , nitrosyl chloride. In other cases these compounds are named as halogenide oxides with the ligands listed alphabetically; for example,  $\text{BiClO}$ , bismuth chloride oxide;  $\text{VCl}_2\text{O}$ , vanadium(IV) dichloride oxide.

**3.1.6.2 Anhydrides.** Anhydrides of inorganic acids are named as oxides; for example,  $\text{N}_2\text{O}_5$ , dinitrogen pentoxide.

**TABLE 3.1** Trivial Names Retained for Acids*Alphabetically by characteristic element.*

|                                               |                                           |                                                             |                                                 |
|-----------------------------------------------|-------------------------------------------|-------------------------------------------------------------|-------------------------------------------------|
| H <sub>3</sub> AsO <sub>4</sub>               | arsenic acid                              | H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>                | diphosphoric acid (or pyro-phosphoric acid)     |
| H <sub>3</sub> AsO <sub>3</sub>               | arsenious acid                            | H <sub>4</sub> P <sub>2</sub> O <sub>8</sub>                | peroxodiphosphoric acid                         |
| H <sub>3</sub> BO <sub>3</sub>                | orthoboric acid (or boric acid)           | (HO) <sub>2</sub> OP                                        | diphosphoric(IV) acid or hypophosphoric acid    |
| HBO <sub>2</sub>                              | metaboric acid                            | (HO) <sub>2</sub> OP                                        |                                                 |
| HBrO <sub>3</sub>                             | bromic acid                               | (HO) <sub>2</sub> P—O                                       | diphosphoric(III,V) acid                        |
| HBrO <sub>2</sub>                             | bromous acid                              | (HO) <sub>2</sub> P—O                                       |                                                 |
| HBrO                                          | hypobromous acid                          | H <sub>2</sub> PHO <sub>3</sub>                             | phosphonic acid                                 |
| H <sub>2</sub> CO <sub>3</sub>                | carbonic acid                             | H <sub>2</sub> P <sub>2</sub> H <sub>2</sub> O <sub>5</sub> | diphosphonic acid                               |
| HOCN                                          | cyanic acid                               | HPH <sub>2</sub> O <sub>2</sub>                             | phosphinic acid (formerly hypophosphorous acid) |
| HNCO                                          | isocyanic acid                            | HReO <sub>4</sub>                                           | perrhenic acid                                  |
| HONC                                          | fulminic acid                             | H <sub>2</sub> ReO <sub>4</sub>                             | rhenic acid                                     |
| HClO <sub>4</sub>                             | perchloric acid                           | H <sub>2</sub> SO <sub>4</sub>                              | sulfuric acid                                   |
| HClO <sub>3</sub>                             | chloric acid                              | H <sub>2</sub> S <sub>2</sub> O <sub>7</sub>                | disulfuric acid                                 |
| HClO <sub>2</sub>                             | chlorous acid                             | H <sub>2</sub> SO <sub>5</sub>                              | peroxomonosulfuric acid                         |
| HClO                                          | hypochlorous acid                         | H <sub>2</sub> S <sub>2</sub> O <sub>3</sub>                | thiosulfuric acid                               |
| H <sub>2</sub> CrO <sub>4</sub>               | chromic acid                              | H <sub>2</sub> S <sub>2</sub> S <sub>6</sub>                | dithionic acid                                  |
| H <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> | dichromic acid                            | H <sub>2</sub> SO <sub>3</sub>                              | sulfurous acid                                  |
| H <sub>5</sub> IO <sub>6</sub>                | orthoperiodic acid                        | H <sub>2</sub> S <sub>2</sub> O <sub>5</sub>                | disulfurous acid                                |
| HIO <sub>4</sub>                              | periodic acid                             | H <sub>2</sub> S <sub>2</sub> O <sub>2</sub>                | thiosulfurous acid                              |
| HIO <sub>3</sub>                              | iodic acid                                | H <sub>2</sub> S <sub>2</sub> O <sub>4</sub>                | dithionous acid                                 |
| HIO                                           | hypoiodous acid                           | H <sub>2</sub> S <sub>x</sub> O <sub>6</sub>                | polythionic acid                                |
| HMnO <sub>4</sub>                             | permanganic acid                          | (x = 3, 4, . . . )                                          | (tri-, tetra-, . . . )                          |
| H <sub>2</sub> MnO <sub>4</sub>               | manganic acid                             | H <sub>2</sub> SO <sub>2</sub>                              | sulfoxylic acid                                 |
| HNO <sub>4</sub>                              | peroxonitric acid                         | HSb(OH) <sub>6</sub>                                        | hexahydroxoantimonic acid                       |
| HNO <sub>3</sub>                              | nitric acid                               | H <sub>2</sub> SeO <sub>4</sub>                             | selenic acid                                    |
| HNO <sub>2</sub>                              | nitrous acid                              | H <sub>2</sub> SeO <sub>3</sub>                             | selenious acid                                  |
| H <sub>2</sub> NO <sub>2</sub>                | nitroxylic acid                           | H <sub>4</sub> SiO <sub>4</sub>                             | orthosilicic acid                               |
| H <sub>2</sub> N <sub>2</sub> O <sub>2</sub>  | hyponitrous acid                          | H <sub>2</sub> SiO <sub>3</sub>                             | metasilicic acid                                |
| HOONO                                         | peroxonitrous acid                        | HTcO <sub>4</sub>                                           | pertechnetic acid                               |
| H <sub>3</sub> PO <sub>4</sub>                | orthophosphoric acid (or phosphoric acid) | H <sub>2</sub> TeO <sub>4</sub>                             | technetic acid                                  |
| HPO <sub>3</sub>                              | metaphosphoric acid                       | H <sub>6</sub> TeO <sub>6</sub>                             | orthotelluric acid                              |
| H <sub>3</sub> PO <sub>5</sub>                | peroxomonophosphoric acid                 |                                                             |                                                 |

**3.1.6.3 Esters.** Esters of inorganic acids are named as the salts; for example, (CH<sub>3</sub>)<sub>2</sub>SO<sub>4</sub>, dimethyl sulfate. However, if it is desired to specify the constitution of the compound, the nomenclature for coordination compounds should be used.

**3.1.6.4 Amides.** Names for amides are derived from the names of the acid radicals (or from the names of acids by replacing acid by amide); for example, SO<sub>2</sub>(NH<sub>2</sub>)<sub>2</sub>, sulfonyl diamide (or sulfuric diamide); NH<sub>2</sub>SO<sub>3</sub>H, sulfamidic acid (or amidosulfuric acid).

**3.1.6.5 Salts.** Salts containing acid hydrogen are named by adding the word hydrogen before the name of the anion (however, see Sec. 3.1.4.1), for example, KH<sub>2</sub>PO<sub>4</sub>, potassium dihydrogen phosphate; NaHCO<sub>3</sub>, sodium hydrogen carbonate (not bicarbonate); NaHPO<sub>3</sub>, sodium hydrogen phosphonate (only one acid hydrogen remaining).

Salts containing O<sup>2-</sup> and HO<sup>-</sup> anions are named oxide and hydroxide, respectively. Anions are cited in alphabetical order which may be different in formulas and names.

*Examples:* FeO(OH), iron(III) hydroxide oxide; VO(SO<sub>4</sub>), vanadium(IV) oxide sulfate.

**3.1.6.6 Multiplicative Prefixes.** The multiplicative prefixes bis, tris, etc., are used with certain anions for indicating stoichiometric proportions when di, tri, etc., have been preempted to designate condensed anions; for example,  $\text{AlK}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ , aluminum potassium bis(sulfate) 12-water (recall that disulfate refers to the anion  $\text{S}_2\text{O}_7^{2-}$ ).

**3.1.6.7 Crystal Structure.** The structure type of crystals may be added in parentheses and in italics after the name; the latter should be in accordance with the structure. When the typename is also the mineral name of the substance itself, italics are not used.

*Examples:*  $\text{MgTiO}_3$ , magnesium titanium trioxide (*ilmenite* type);  $\text{FeTiO}_3$ , iron(II) titanium trioxide (*ilmenite*).

### 3.1.7 Coordination Compounds

**3.1.7.1 Naming a Coordination Compound.** To name a coordination compound, the names of the ligands are attached directly in front of the name of the central atom. The ligands are listed in alphabetical order regardless of the number of each and with the name of a ligand treated as a unit. Thus “diammine” is listed under “a” and “dimethylamine” under “d.” The oxidation number of the central atom is stated last by either the oxidation number or charge number.

**3.1.7.2 Anionic Ligands.** Whether inorganic or organic, the names for anionic ligands end in -o (eliding the final -e, if present, in the anion name). Enclosing marks are required for inorganic anionic ligands containing numerical prefixes, and for thio, seleno, and telluro analogs of oxo anions containing more than one atom.

If the coordination entity is negatively charged, the cations paired with the complex anion (with -ate ending) are listed first. If the entity is positively charged, the anions paired with the complex cation are listed immediately afterward.

The following anions do not follow the nomenclature rules:

|                   |                    |                         |                               |
|-------------------|--------------------|-------------------------|-------------------------------|
| $\text{F}^-$      | fluoro             | $\text{HO}_2^-$         | hydrogen peroxo               |
| $\text{Cl}^-$     | chloro             | $\text{S}^{2-}$         | thio (only for single sulfur) |
| $\text{Br}^-$     | bromo              | $\text{S}_2^{2-}$       | disulfido                     |
| $\text{I}^-$      | iodo               | $\text{HS}^-$           | mercapto                      |
| $\text{O}^{2-}$   | oxo                | $\text{CN}^-$           | ciano                         |
| $\text{H}^-$      | hydrido (or hydro) | $\text{CH}_2\text{O}^-$ | methoxo or methanolato        |
| $\text{OH}^-$     | hydroxo            | $\text{CH}_2\text{S}^-$ | methylthio or methanethiolato |
| $\text{O}_2^{2-}$ | peroxo             |                         |                               |

**3.1.7.3 Neutral and Cationic Ligands.** Neutral and cationic ligands are used without change in name and are set off with enclosing marks. Water and ammonia, as neutral ligands, are called “aqua” and “ammine,” respectively. The groups NO and CO, when linked directly to a metal atom, are called nitrosyl and carbonyl, respectively.

**3.1.7.4 Attachment Points of Ligands.** The different points of attachment of a ligand are denoted by adding italicized symbol(s) for the atom or atoms through which the attachment occurs at the end of the name of the ligand; e.g., glycine-*N* or glycinate-*O,N*. If the same element is involved in different possible coordination sites, the position in the chain or ring to which the element is attached is indicated by numerical superscripts: e.g., tartrato(3-)- $\text{O}^1, \text{O}^2$ , or tartrato(4-)- $\text{O}^2, \text{O}^3$  or tartrato(2-)- $\text{O}^1, \text{O}^4$ .

**3.1.7.5 Abbreviations for Ligand Names.** Except for certain hydrocarbon radicals, for ligand (L) and metal (M), and a few with H, all abbreviations are in lowercase letters and do not involve hyphens. In formulas, the ligand abbreviation is set off with parentheses. Some common abbreviations are

|                     |                                                      |                    |                                           |
|---------------------|------------------------------------------------------|--------------------|-------------------------------------------|
| Ac                  | acetyl                                               | en                 | ethylenediamine                           |
| acac                | acetylacetonato                                      | Him                | imidazole                                 |
| Hacac               | acetylacetone                                        | H <sub>2</sub> ida | iminodiacetic acid                        |
| Hba                 | benzoylacetone                                       | Me                 | methyl                                    |
| Bzl                 | benzyl                                               | H <sub>3</sub> nta | nitrilotriacetic acid                     |
| Hbg                 | biguanide                                            | nbd                | norbornadiene                             |
| bpy                 | 2,2'-bipyridine                                      | ox                 | oxalato(2-) from parent H <sub>2</sub> ox |
| Bu                  | butyl                                                | phen               | 1,10-phenanthroline                       |
| Cy                  | cyclohexyl                                           | Ph                 | phenyl                                    |
| D <sub>2</sub> dea  | diethanolamine                                       | pip                | piperidine                                |
| dien                | diethylenetriamine                                   | Pr                 | propyl                                    |
| dmf                 | dimethylformamide                                    | pn                 | propylenediamine                          |
| H <sub>2</sub> dmg  | dimethylglyoxime                                     | Hpz                | pyrazole                                  |
| dmg                 | dimethylglyoximato(2-)                               | py                 | pyridine                                  |
| Hdmg                | dimethylglyoximato(1-)                               | thf                | tetrahydrofuran                           |
| dmsO                | dimethylsulfoxide                                    | tu                 | thiourea                                  |
| Et                  | ethyl                                                | H <sub>3</sub> tea | triethanolamine                           |
| H <sub>4</sub> edta | ethylenediaminetetraacetic acid                      | tren               | 2,2',2''-triiminotriethylamine            |
| Hedta, edta         | coordinated ions derived<br>from H <sub>4</sub> edta | trien              | triethylenetetraamine                     |
| Hea                 | ethanolamine                                         | tn                 | trimethylenediamine                       |
|                     |                                                      | ur                 | urea                                      |

*Examples:* Li[B(NH<sub>2</sub>)<sub>4</sub>], lithium tetraamidoborate(1-) or lithium tetraamidoborate(III); [Co(NH<sub>3</sub>)<sub>5</sub>Cl]Cl<sub>3</sub>, pentaamminechlorocobalt(III) chloride or pentaamminechlorocobalt(2+) chloride; K<sub>3</sub>[Fe(CN)<sub>5</sub>CO], potassium carbonylpentacyanoferrate(II) or potassium carbonylpentacyanoferrate(3-); [Mn{C<sub>6</sub>H<sub>4</sub>(O)(COO)}<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>]<sup>-</sup>, tetraaquabis[salicylato(2-)]manganate(III) ion; [Ni(C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>)<sub>2</sub>] or [Ni(dmg)] which can be named bis-(2,3-butanedione dioximato)nickel(II) or bis[dimethylglyoximato(2-)]nickel(II).

### 3.1.8 Addition Compounds

The names of addition compounds are formed by connecting the names of individual compounds by a dash (—) and indicating the numbers of molecules in the name by Arabic numerals separated by the solidus (diagonal slash). All molecules are cited in order of increasing number; those having the same number are cited in alphabetic order. However, boron compounds and water are always cited last and in that order.

*Examples:* 3CdSO<sub>4</sub> · 8H<sub>2</sub>O, cadmium sulfate—water (3/8); Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> · K<sub>2</sub>SO<sub>4</sub> · 24H<sub>2</sub>O, aluminum sulfate—potassium sulfate—water (1/1/24); AlCl<sub>3</sub> · 4C<sub>2</sub>H<sub>5</sub>OH, aluminum chloride—ethanol (1/4).

## 3.2 PHYSICAL PROPERTIES OF PURE SUBSTANCES

**TABLE 3.2** Physical Constants of Inorganic Compounds

*Names* follow the IUPAC Nomenclature. Solvates are listed under the entry for the anhydrous salt. Acids are entered under Hydrogen and acid salts are entered as a subentry under hydrogen.

*Formula weights* are based upon the International Atomic Weights of 1993 and are computed to the nearest hundredth when justified. The actual significant figures are given in the atomic weights of the individual elements.

Each element that has neither a stable isotope nor a characteristic natural isotopic composition is represented in this table by one of that element's commonly known radioisotopes identified by mass number and relative atomic mass.

*Density* values are given at room temperature unless otherwise indicated by the superscript figure; for example,  $2.487^{15}$  indicates a density of 2.487 g/cm<sup>3</sup> for the substance at 15°C. A superscript 20 over a subscript 4 indicates a density at 20°C relative to that of water at 4°C. For gases the values are given as grams per liter (g/L).

*Melting point* is recorded in a certain case as 250 d and in some other cases as d 250, the distinction being made in this manner to indicate that the former is a melting point with decomposition at 250°C while in the latter decomposition only occurs at 250°C and higher temperatures. Where a value such as  $-6\text{H}_2\text{O}$ , 150 is given it indicates a loss of 6 moles of water per formula weight of the compound at a temperature of 150°C. For hydrates the temperature stated represents the compound melting in its water of hydration.

*Boiling point* is given at atmospheric pressure (760 mm of mercury or 101 325 Pa) unless otherwise indicated; thus  $82^{15\text{mm}}$  indicates that the boiling point is 82°C when the pressure is 15 mm of mercury. Also, subl 550 indicates that the compound sublimates at 550°C. Occasionally decomposition products are mentioned.

*Solubility* is given in parts by weight (of the formula weight) per 100 parts by weight of the solvent (i.e., percent by weight) and at room temperature. Another unit frequently used is grams per 100 mL of solvent (mL per 100 mL for liquids and gases). The symbols of the common mineral acids represent aqueous solutions of these acids.

### Abbreviations Used in the Table

|                                  |                      |
|----------------------------------|----------------------|
| a, acid                          | h, hot               |
| abs, absolute                    | hex, hexagonal       |
| abs alc, anhydrous ethanol       | HOAc, acetic acid    |
| acet, acetone                    | i, insoluble         |
| alk, alkali (aq NaOH or KOH)     | ign, ignites         |
| anhyd, anhydrous                 | L, liter             |
| aq, aqueous                      | lq, liquid           |
| aq reg, aqua regia               | MeOH, methanol       |
| atm, atmosphere                  | min, mineral         |
| BuOH, butanol                    | mL, milliliter       |
| bz, benzene                      | org, organic         |
| c, solid state                   | oxid, oxidizing      |
| ca., approximately               | PE, petroleum ether  |
| chl, chloroform                  | pyr, pyridine        |
| conc, concentrated               | s, soluble           |
| cub, cubic                       | satd, saturated      |
| d, decomposes                    | sl, slightly         |
| dil, dilute                      | soln, solution       |
| disprop, disproportionates       | solv, solvent(s)     |
| EtOAc, ethyl acetate             | subl, sublimates     |
| eth, diethyl ether               | sulf, sulfides       |
| EtOH, 95% ethanol                | tart, tartrate       |
| expl, explodes                   | THF, tetrahydrofuran |
| fcc, face-centered cubic         | v, very              |
| fctetr, face-centered tetragonal | vac, vacuum          |
| FP, flash point                  | viol, violently      |
| fum, fuming                      | volat, volatilizes   |
| fus, fusion, fuses               | <, less than         |
| g, gas, gram                     | >, greater than      |
| glyc, glycerol                   |                      |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                        | Formula                                                                  | Formula weight | Density                           | Melting point,<br>°C                    | Boiling point,<br>°C      | Solubility in<br>100 parts solvent                                                      |
|-----------------------------|--------------------------------------------------------------------------|----------------|-----------------------------------|-----------------------------------------|---------------------------|-----------------------------------------------------------------------------------------|
| Actinium-227                | Ac                                                                       | 227.0278       | 10.07                             | 1050(50)                                | ca. 3200                  | d aq; s acids                                                                           |
| bromide                     | AcBr <sub>3</sub>                                                        | 466.74         | 5.85                              | subl 800                                |                           | s aq                                                                                    |
| Aluminum                    | Al                                                                       | 26.981539      | 2.70                              | 660.323                                 | 2518                      | s HCl, H <sub>2</sub> SO <sub>4</sub> , alk                                             |
| acetylacetonate             | Al(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub>           | 324.31         | 1.27                              | 190–193                                 | 315                       | i aq; v s alc; s bz, eth                                                                |
| ammonium bis(sulfate)       | AlNH <sub>4</sub> (SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O   | 453.33         | 1.65                              | anhyd > 280                             |                           | 14.3 g/100 mL aq; s glyc; i alc                                                         |
| 12-water                    |                                                                          |                |                                   |                                         |                           |                                                                                         |
| antimonide                  | AlSb                                                                     | 148.74         | 4.26                              | 1060                                    |                           |                                                                                         |
| arsenide                    | AlAs                                                                     | 101.90         | 3.76                              | 1740                                    |                           |                                                                                         |
| bis(acetylsalicylate)       | Al(OOCC <sub>6</sub> H <sub>4</sub> OCOCH <sub>3</sub> ) <sub>2</sub> OH | 402.30         |                                   |                                         |                           | v sl s aq, alc, eth                                                                     |
| borate (2/1)                | 2Al <sub>2</sub> O <sub>3</sub> · B <sub>2</sub> O <sub>3</sub>          | 273.54         |                                   | ca. 1050                                |                           | i aq                                                                                    |
| bromide                     | AlBr <sub>3</sub>                                                        | 266.69         | 3.205 <sup>18</sup> <sub>0</sub>  | 97.5                                    | subl 253                  | d (viol) aq; s alc, acet, bz, CS <sub>2</sub>                                           |
| butoxide, sec-              | Al(C <sub>4</sub> H <sub>9</sub> O) <sub>3</sub>                         | 246.33         | 0.967                             |                                         | 200–206 <sup>30mm</sup>   | FP 27; v s org solv                                                                     |
| butoxide, tert-             | Al(C <sub>4</sub> H <sub>9</sub> O) <sub>3</sub>                         | 246.33         | 1.025 <sup>20</sup> <sub>0</sub>  |                                         | subl 180                  | v s org solv                                                                            |
| carbide (4/3)               | Al <sub>4</sub> C <sub>3</sub>                                           | 143.96         | 2.360                             | 2100                                    | d > 2200 <sup>400mm</sup> | d aq; fire hazard                                                                       |
| chlorate                    | Al(ClO <sub>3</sub> ) <sub>3</sub>                                       | 277.35         |                                   |                                         |                           | v s aq; s alc                                                                           |
| chloride                    | AlCl <sub>3</sub>                                                        | 133.34         | 2.440 <sup>25</sup>               | 192.6                                   | subl 181.1                | g/100 mL: 70 aq (viol), 100 <sup>12</sup> abs<br>alc; s CCl <sub>4</sub> , eth; sl s bz |
| ethoxide                    | Al(C <sub>2</sub> H <sub>5</sub> O) <sub>3</sub>                         | 162.16         | 1.142 <sup>20</sup> <sub>0</sub>  | 140                                     | 205 <sup>14mm</sup>       | s hot aq d; v sl s alc, eth                                                             |
| fluoride                    | AlF <sub>3</sub>                                                         | 83.98          | 2.882 <sup>25</sup> <sub>4</sub>  | 1090                                    | subl 1272                 | 0.56 aq; i a, alk, alc, acet                                                            |
| hydroxide                   | Al(OH) <sub>3</sub>                                                      | 78.01          | 2.42                              | to Al <sub>2</sub> O <sub>3</sub> , 300 |                           | i aq; s acids, alkalis                                                                  |
| iodide                      | AlI <sub>3</sub>                                                         | 407.69         | 3.98 <sup>17</sup>                | 191.0                                   | 382                       | d aq; s alc, eth, CS <sub>2</sub>                                                       |
| isopropoxide                | Al(C <sub>3</sub> H <sub>7</sub> O) <sub>3</sub>                         | 204.25         | 1.0346 <sup>20</sup> <sub>0</sub> | 118.5                                   | 135 <sup>10mm</sup>       | d aq; s alc, bz, chl, PE                                                                |
| methoxide                   | Al(CH <sub>3</sub> O) <sub>3</sub>                                       | 72.07          |                                   | 0                                       | 130                       |                                                                                         |
| nitrate 9-water             | Al(NO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O                    | 375.13         | 1.72                              | 73                                      | d 135                     | g/100 mL: 64 aq, 100 alc; s acet                                                        |
| nitride                     | AlN                                                                      | 40.99          | 3.05                              | d 2517                                  |                           | d aq, acid, alkali                                                                      |
| oxide (alpha-)              | AlO <sub>3</sub>                                                         | 101.96         | 3.97                              | 2054(6)                                 | 2980                      | i aq; v sl s a, alk                                                                     |
| perchlorate 6-water         | Al(ClO <sub>4</sub> ) <sub>3</sub> · 6H <sub>2</sub> O                   | 433.43         | 2.020                             | 120.8                                   | anhyd 178                 | 133 g/100 mL <sup>20</sup> aq                                                           |
| phenoxide                   | Al(C <sub>6</sub> H <sub>5</sub> O) <sub>3</sub>                         | 306.27         | 1.23                              | d 265                                   |                           | d aq; s alc, chl, eth                                                                   |
| phosphate                   | AlPO <sub>4</sub>                                                        | 121.95         | 2.56                              | > 1460                                  |                           | i aq; sl s a                                                                            |
| phosphide                   | AlP                                                                      | 57.96          | 2.85 <sup>45</sup> <sub>5</sub>   | 2550                                    |                           | d aq                                                                                    |
| phosphinate (hypophosphite) | Al(H <sub>2</sub> PO <sub>2</sub> ) <sub>3</sub>                         | 221.94         |                                   | d to PH <sub>3</sub> , 220              |                           | i aq; s HCl, warm alkali                                                                |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                                 | Formula                                                                | Formula weight | Density                                             | Melting point,<br>°C         | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                       |
|--------------------------------------|------------------------------------------------------------------------|----------------|-----------------------------------------------------|------------------------------|----------------------|--------------------------------------------------------------------------|
| Aluminum ( <i>continued</i> )        |                                                                        |                |                                                     |                              |                      |                                                                          |
| potassium bis(sulfate)<br>12-water   | AlK(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O                | 474.39         | 1.757 <sup>20</sup>                                 | − 9H <sub>2</sub> O, 92      | anhyd, 200           | 11.4 g/100 mL aq; v s glyc; i alc                                        |
| propoxide                            | Al(C <sub>3</sub> H <sub>7</sub> O) <sub>3</sub>                       | 204.25         | 1.0578 <sup>20</sup> <sub>0</sub>                   | 106                          | 248 <sup>14mm</sup>  | d aq; s alc                                                              |
| selenide                             | Al <sub>2</sub> Se <sub>3</sub>                                        | 290.84         | 3.437 <sup>20</sup> <sub>4</sub>                    | 947                          |                      | d aq, acid                                                               |
| silicon oxide (1/1)                  | Al <sub>2</sub> O <sub>3</sub> · SiO <sub>2</sub>                      | 162.05         | 3.247                                               |                              |                      | i aq; d HF; s fused alkali                                               |
| sodium bis(sulfate)<br>12-water      | AlNa(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O               | 458.28         | 1.675 <sup>20</sup>                                 | 61                           |                      | 110 g/100 mL <sup>15</sup> aq; i alc                                     |
| stearate                             | Al(C <sub>18</sub> H <sub>35</sub> O <sub>2</sub> ) <sub>3</sub>       | 877.41         | 1.070                                               | 117–120                      |                      | i aq, alc; s bz, alk                                                     |
| sulfate                              | Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                        | 342.15         | 1.61                                                | 770 d                        |                      | 36.4 g/100 mL <sup>20</sup> aq; sl s alc                                 |
| sulfate 18-water                     | Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 18H <sub>2</sub> O   | 666.46         | 1.69 <sup>17</sup>                                  | d 86.5                       |                      | 87 g/100 mL <sup>0</sup> aq; i alc                                       |
| sulfide                              | Al <sub>2</sub> S <sub>3</sub>                                         | 150.16         | 2.20 <sup>13</sup>                                  | 1097                         | subl 1500            | hyd aq; s acid                                                           |
| tetrahydridoborate                   | Al(BH <sub>4</sub> ) <sub>3</sub>                                      | 71.53          |                                                     | − 64.5                       | 44.5                 | d aq; ign air; expl in O <sub>2</sub> , 20                               |
| Americium                            | Am                                                                     | 243            | 12                                                  | 1176                         | 2011                 | s a                                                                      |
| Ammonia                              | NH <sub>3</sub>                                                        | 17.03          | lq: 0.6818 at bp<br>g: 0.6175 <sup>15, 7.2atm</sup> | − 77.75                      | − 33.35              | g/100 mL: 34 aq; 13.2 alc; s eth,<br>organic solvents                    |
| Ammonium acetate                     | NH <sub>4</sub> C <sub>2</sub> H <sub>3</sub> O <sub>2</sub>           | 77.08          | 1.17 <sup>20</sup>                                  | 114                          | d                    | g/100 mL: 148 <sup>4</sup> aq, 7.9 <sup>15</sup> MeOH; s<br>alc          |
| amidosulfate                         | NH <sub>4</sub> SO <sub>3</sub> NH <sub>2</sub>                        | 114.13         |                                                     | 131                          | d 160                | v s aq; sl s alc                                                         |
| benzoate                             | NH <sub>4</sub> C <sub>6</sub> H <sub>5</sub> O <sub>2</sub>           | 139.15         | 1.260                                               | 198                          | subl 160             | g/100 mL: 20 <sup>15</sup> aq, 2.8 alc; s glyc                           |
| bromide                              | NH <sub>4</sub> Br                                                     | 97.94          | 2.429                                               | 452 (subl under<br>pressure) | d 397 vacuo          | 76 g/100 mL <sup>20</sup> aq; v s acet, alc, eth                         |
| calcium arsenate 6-water             | NH <sub>4</sub> CaAsO <sub>4</sub> · 6H <sub>2</sub> O                 | 305.13         | 1.905 <sup>15</sup>                                 | d 140                        |                      | 0.02 aq; s NH <sub>4</sub> Cl                                            |
| carbamate                            | NH <sub>4</sub> COONH <sub>2</sub>                                     | 78.07          |                                                     | subl 60                      |                      | v s aq; sl s alc; i eth                                                  |
| carbonate 1-water                    | (NH <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub> · H <sub>2</sub> O     | 114.10         |                                                     | volatilizes 60               |                      | v s aq; i alc                                                            |
| chloride                             | NH <sub>4</sub> Cl                                                     | 53.49          | 1.5274 <sup>25</sup>                                | 237.8                        | 520                  | g/100 mL: 26 <sup>15</sup> aq, 0.6 <sup>19</sup> abs alc; i<br>acet, eth |
| chromate(VI)                         | (NH <sub>4</sub> ) <sub>2</sub> CrO <sub>4</sub>                       | 152.07         | 1.91 <sup>12</sup>                                  | d 185                        |                      | 34 g/100 mL <sup>20</sup> aq; sl s MeOH                                  |
| chromium(III) bissulfate<br>12-water | NH <sub>4</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O | 478.34         | 1.72                                                | 94 d                         |                      | 7.2 g/100 mL <sup>0</sup> aq                                             |
| copper(II) tetrachloride<br>2-water  | (NH <sub>4</sub> ) <sub>2</sub> CuCl <sub>4</sub> · 2H <sub>2</sub> O  | 277.46         | 1.993                                               | anhyd, 110                   | d >120               | 40.3 g/100 mL <sup>20</sup> aq; s alc                                    |



|                              |                                                                       |         |                     |                                            |       |                                                     |
|------------------------------|-----------------------------------------------------------------------|---------|---------------------|--------------------------------------------|-------|-----------------------------------------------------|
| cyanide                      | $\text{NH}_4\text{CN}$                                                | 44.06   | 1.10                | d 36                                       |       | v s aq, alc                                         |
| dichromate(VI)               | $(\text{NH}_4)_2\text{Cr}_2\text{O}_7$                                | 252.07  | 2.155               | d 180 to $\text{Cr}_2\text{O}_3$           |       | 35.6 g/100 mL <sup>20</sup> aq; s alc;<br>flammable |
| dihydrogen arsenate          | $\text{NH}_4\text{H}_2\text{AsO}_4$                                   | 158.97  | 2.311               | d 300                                      |       | v s aq                                              |
| dihydrogen phosphate         | $\text{NH}_4\text{H}_2\text{PO}_4$                                    | 115.03  | 1.803 <sup>19</sup> | d 190                                      |       | 37 g/100 mL <sup>20</sup> aq; sl s alc; i acet      |
| disulfatocobaltate(II)       | $(\text{NH}_4)_2[\text{Co}(\text{SO}_4)_2] \cdot 6\text{H}_2\text{O}$ | 395.23  | 1.902               |                                            |       | 18 g/100 mL <sup>20</sup> aq; v sl s alc            |
| 6-water                      |                                                                       |         |                     |                                            |       |                                                     |
| disulfatoferrate(II) 6-water | $(\text{NH}_4)_2[\text{Fe}(\text{SO}_4)_2] \cdot 6\text{H}_2\text{O}$ | 392.14  | 1.864               | d 100                                      |       | 36.4 g/100 mL <sup>20</sup> aq; i alc               |
| disulfatoferrate(III)        | $\text{NH}_4[\text{Fe}(\text{SO}_4)_2] \cdot 12\text{H}_2\text{O}$    | 482.19  | 1.71                | 39–41                                      | d 230 | 124 g/100 mL aq                                     |
| 12-water                     |                                                                       |         |                     |                                            |       |                                                     |
| disulfatonickelate(II)       | $(\text{NH}_4)_2[\text{Ni}(\text{SO}_4)_2] \cdot 6\text{H}_2\text{O}$ | 395.00  | 1.923               |                                            |       | 8.95 g/100 mL <sup>20</sup> aq                      |
| 6-water                      |                                                                       |         |                     |                                            |       |                                                     |
| dithiocarbamate              | $\text{NH}_4\text{S}(\text{C}=\text{S})\text{NH}_2$                   | 110.20  | 1.451 <sup>20</sup> | 99 d                                       |       | v s aq; s alc; sl s eth                             |
| diuranate(VI)                | $(\text{NH}_4)_2\text{U}_2\text{O}_7$                                 | 624.22  |                     |                                            |       | v sl s aq, alk; s acids                             |
| fluoride                     | $\text{NH}_4\text{F}$                                                 | 37.04   | 1.009 <sup>25</sup> | d to $\text{NH}_3 + \text{HF}$             |       | 100 g/100 mL <sup>0</sup> aq; s alc                 |
| formate                      | $\text{NH}_4\text{OOCH}$                                              | 63.06   | 1.27                | 116                                        | d 180 | 143 g/100 mL <sup>20</sup> aq; s alc, eth           |
| heptamolybdate(VI)(6–)       | $(\text{NH}_4)_2\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$   | 1235.86 | 2.498               | anhyd 90                                   | d 190 | 43 g/100 mL aq; s acids; i alc                      |
| 4-water                      |                                                                       |         |                     |                                            |       |                                                     |
| hexachloropalladate(IV)      | $(\text{NH}_4)_2[\text{PdCl}_6]$                                      | 355.20  | 2.418               | d                                          |       | sl s aq                                             |
| hexachloroplatinate(IV)      | $(\text{NH}_4)_2[\text{PtCl}_6]$                                      | 443.87  | 3.065               | d 380                                      |       | 0.5 aq                                              |
| hexadecanoate                | $\text{NH}_4\text{OOC}(\text{CH}_2)_{14}\text{CH}_3$                  | 273.45  |                     | 21–22                                      |       | s aq; sl s bz; i alc, acet                          |
| hexafluoroaluminate(3–)      | $(\text{NH}_4)_3[\text{AlF}_6]$                                       | 195.09  | 1.78                | d > 100                                    |       | v s aq                                              |
| hexafluorogallate            | $(\text{NH}_4)_3\text{GaF}_6$                                         | 237.83  | 2.10                | d 200                                      |       |                                                     |
| hexafluorogermanate          | $(\text{NH}_4)_3\text{GeF}_6$                                         | 222.68  | 2.564               | 380                                        | subl  | s aq; i eth                                         |
| hexafluorophosphate          | $\text{NH}_4[\text{PF}_6]$                                            | 163.00  | 2.180 <sup>18</sup> | d 68                                       |       | 74.8 g/100 mL <sup>20</sup> aq; s alc, acet         |
| hexafluorosilicate           | $(\text{NH}_4)_2[\text{SiF}_6]$                                       | 178.15  | 2.011               | d                                          |       | 18.6 g/100 mL <sup>20</sup> aq; i alc, acet         |
| hexanitratocerate(IV)        | $(\text{NH}_4)_2[\text{Ce}(\text{NO}_3)_6]$                           | 548.22  |                     |                                            |       | 135 g/100 mL <sup>20</sup> aq; s alc, HNO           |
| hydrogen carbonate           | $\text{NH}_4\text{HCO}_3$                                             | 79.06   | 1.586               | 107 (rapid heating)                        |       | g/100 mL: 17.4 <sup>20</sup> aq, 10 glyc            |
| hydrogen citrate             | $(\text{NH}_4)_2\text{HC}_6\text{H}_5\text{O}_7$                      | 226.19  | 1.48                |                                            |       | 100 g/100 mL aq; sl s alc                           |
| hydrogen difluoride          | $\text{NH}_4\text{HF}_2$                                              | 57.04   | 1.51                | 124.6                                      | 240 d | v s aq; sl s alc                                    |
| hydrogen oxalate hydrate     | $\text{NH}_4\text{HC}_2\text{O}_4 \cdot \text{H}_2\text{O}$           | 125.08  | 1.556               | anhyd, 170                                 |       | s aq, alc; i bz, eth                                |
| hydrogen phosphate           | $(\text{NH}_4)_2\text{HPO}_4$                                         | 132.06  | 1.619               | d 155                                      |       | 69 g/100 mL <sup>20</sup> aq; i alc, acet           |
| hydrogen sulfate             | $\text{NH}_4\text{HSO}_4$                                             | 115.11  | 1.78                | 146.9                                      | d 350 | 100 g/100 mL aq; i alc, acet                        |
| hydrogen sulfide             | $\text{NH}_4\text{HS}$                                                | 51.11   | 1.17                | d 25 to $\text{NH}_3 + \text{H}_2\text{S}$ |       | 128 g/100 mL <sup>0</sup> aq; s glyc; i alc, acet   |
| hydrogen sulfite             | $\text{NH}_4\text{HSO}_3$                                             | 99.11   | 2.03                | subl 150 in $\text{N}_2$                   |       | 267 g/100 mL <sup>10</sup> aq                       |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                                  | Formula                                                                                 | Formula weight | Density             | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                                      |
|---------------------------------------|-----------------------------------------------------------------------------------------|----------------|---------------------|----------------------|----------------------|-----------------------------------------------------------------------------------------|
| Ammonium acetate ( <i>continued</i> ) |                                                                                         |                |                     |                      |                      |                                                                                         |
| hydrogen (±)tartrate                  | NH <sub>4</sub> HC <sub>4</sub> H <sub>4</sub> O <sub>6</sub>                           | 167.12         | 1.68                | d 200                |                      | 2.2 <sup>15</sup> aq; i alc                                                             |
| hydroxide                             | NH <sub>4</sub> OH                                                                      | 35.05          |                     | − 77                 |                      | 49% dissolved NH <sub>3</sub>                                                           |
| hypophosphite                         | NH <sub>4</sub> H <sub>2</sub> PO <sub>2</sub>                                          | 83.03          |                     | d                    |                      | v s aq; sl s alc; i acet                                                                |
| iodate                                | NH <sub>4</sub> IO <sub>3</sub>                                                         | 192.94         | 3.309               | d 150                |                      | 2.6 <sup>15</sup> aq                                                                    |
| iodide                                | NH <sub>4</sub> I                                                                       | 144.94         | 2.514 <sup>25</sup> | subl 551             | 220 vacuo            | 167 g/100 mL <sup>20</sup> aq; v s alc, acet                                            |
| lactate                               | NH <sub>4</sub> C <sub>3</sub> H <sub>5</sub> O <sub>3</sub>                            | 107.11         | 1.2 <sup>15</sup>   | 92                   |                      | v s aq, alc, glyc; i acet, eth                                                          |
| magnesium arsenate<br>6-water         | NH <sub>4</sub> MgAsO <sub>4</sub> · 6H <sub>2</sub> O                                  | 289.36         | 1.923               | d                    |                      | 0.038 <sup>20</sup> aq                                                                  |
| molybdate(VI)(2−)                     | (NH <sub>4</sub> ) <sub>2</sub> MoO <sub>4</sub>                                        | 196.04         | 2.276 <sup>25</sup> | d                    |                      | s acids                                                                                 |
| nitrate                               | NH <sub>4</sub> NO <sub>3</sub>                                                         | 80.04          | 1.725 <sup>25</sup> | 169.6                | d 210                | g/100 mL: 192 <sup>20</sup> aq; 3.8 <sup>20</sup> alc; 17 <sup>20</sup><br>MeOH; s acet |
| octadecanoate                         | NH <sub>4</sub> OOC(CH <sub>2</sub> ) <sub>16</sub> CH <sub>3</sub>                     | 301.50         |                     | 21–22                |                      | sl s aq; s alc; i acet                                                                  |
| octanoate                             | NH <sub>4</sub> OOC(CH <sub>2</sub> ) <sub>6</sub> CH <sub>3</sub>                      | 161.24         |                     | d on standing        |                      | v s aq, alc, acet; sl s eth                                                             |
| oxalate hydrate                       | (NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> O <sub>4</sub> · H <sub>2</sub> O        | 142.11         | 1.50                | d 70                 |                      | 5.1 <sup>20</sup> aq; s alc                                                             |
| oxodioxalatotitanate(IV)              | (NH <sub>4</sub> ) <sub>2</sub> TiO(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub>        | 276.02         |                     |                      |                      | v s aq                                                                                  |
| perchlorate                           | NH <sub>4</sub> ClO <sub>4</sub>                                                        | 117.49         | 1.95                | d 240                |                      | g/100 mL <sup>25</sup> : 21.9 aq, 1.49 EtOH,<br>0.014 BuOH, 0.029 EtOAc                 |
| permanganate                          | NH <sub>4</sub> MnO <sub>4</sub>                                                        | 136.97         | 2.208 <sup>10</sup> | explodes, 110        |                      | 0.8 <sup>15</sup> aq                                                                    |
| peroxodisulfate                       | (NH <sub>4</sub> ) <sub>2</sub> S <sub>2</sub> O <sub>8</sub>                           | 228.20         | 1.982               | d 120                | expl 180             | 58 g/100 mL <sup>0</sup> aq                                                             |
| phosphinate                           | NH <sub>4</sub> PH <sub>2</sub> O <sub>2</sub>                                          | 83.04          | 1.634               | 200                  | d 240                | g/100 mL: 100 aq, 5 alc; i acet                                                         |
| phosphomolybdate<br>hydrate           | (NH <sub>4</sub> ) <sub>3</sub> PO <sub>4</sub> · 12MoO <sub>3</sub> · H <sub>2</sub> O | 1894.36        |                     | d                    |                      | sl s aq                                                                                 |
| picrate                               | NH <sub>4</sub> C <sub>6</sub> H <sub>2</sub> N <sub>3</sub> O <sub>7</sub>             | 246.14         | 1.719               | d                    | expl 423             | 1.1 <sup>20</sup> aq; sl s alc                                                          |
| selenate(VI)                          | (NH <sub>4</sub> ) <sub>2</sub> SeO <sub>4</sub>                                        | 179.04         | 2.193 <sup>20</sup> | d                    |                      | 117 g/100 mL <sup>7</sup> aq; s HOAC; i alc                                             |
| stearate                              | NH <sub>4</sub> C <sub>18</sub> H <sub>35</sub> O <sub>2</sub>                          | 301.51         | 0.89                | 22                   |                      | sl s aq, bz; s alc; i acet                                                              |
| sulfamate                             | NH <sub>4</sub> NH <sub>2</sub> SO <sub>3</sub>                                         | 114.13         |                     | 131                  | d 160                | v s aq; sl s alc                                                                        |
| sulfate                               | (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>                                         | 132.14         | 1.769 <sup>20</sup> | d > 280              |                      | 43.5 g/100 mL <sup>20</sup> aq; i alc, acet                                             |
| sulfide                               | (NH <sub>4</sub> ) <sub>2</sub> S                                                       | 68.14          |                     | d ≈ 0                |                      | v s aq; s alc, alk                                                                      |
| sulfite hydrate                       | (NH <sub>4</sub> ) <sub>2</sub> SO <sub>3</sub> · H <sub>2</sub> O                      | 134.16         | 1.41                | d 60                 |                      | 75 g/100 mL <sup>20</sup> aq; i alc, acet                                               |
| (±)tartrate                           | (NH <sub>4</sub> ) <sub>2</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub>            | 184.15         | 1.601               | d                    |                      | 58 g/100 mL <sup>15</sup> aq; sl s alc                                                  |
| tetraborate 4-water                   | (NH <sub>4</sub> ) <sub>2</sub> B <sub>4</sub> O <sub>7</sub> · 4H <sub>2</sub> O       | 263.44         |                     |                      |                      | s aq; i alc                                                                             |

|                           |                                                 |             |                                   |                        |                    |                                                                        |
|---------------------------|-------------------------------------------------|-------------|-----------------------------------|------------------------|--------------------|------------------------------------------------------------------------|
| tetrachloroaluminate      | $\text{NH}_4[\text{AlCl}_4]$                    | 186.83      |                                   | 304                    |                    | s aq, eth                                                              |
| tetrachloropalladate(II)  | $(\text{NH}_4)_2[\text{PdCl}_4]$                | 284.29      | 2.170                             | d                      |                    | v s aq; i abs alc                                                      |
| tetrachloroplatinate(II)  | $(\text{NH}_4)_2[\text{PtCl}_4]$                | 372.97      | 2.936                             | 140 d                  |                    | s aq; i alc                                                            |
| tetrachlorozincate        | $(\text{NH}_4)_2[\text{ZnCl}_4]$                | 243.28      | 1.879                             | 150 d                  | subl 341           | v s aq                                                                 |
| tetrafluoroborate         | $\text{NH}_4[\text{BF}_4]$                      | 104.84      | 1.871                             | subl                   |                    | 25 g/100 mL <sup>16</sup> aq                                           |
| thiocyanate               | $\text{NH}_4\text{SCN}$                         | 76.12       | 1.305                             | 149.6                  | d 170              | 128 g/100 mL <sup>0</sup> aq; v s alc; s acet                          |
| thiosulfate               | $(\text{NH}_4)_2\text{S}_2\text{O}_3$           | 148.21      | 1.679                             | d 150                  |                    | 2.15 <sup>15</sup> aq; i alc, eth                                      |
| vanadate(V)(1–)           | $\text{NH}_4\text{VO}_3$                        | 116.98      | 2.326                             | d 200                  |                    | 0.48 <sup>20</sup> aq                                                  |
| Antimony                  | Sb                                              | 121.760(1)  | 6.697 <sup>25</sup>               | 630.7                  | 1587               | s hot conc $\text{H}_2\text{SO}_4$ , aqua regia                        |
| arsenide                  | SbAs                                            | 196.68      | 6.0                               | ≈680                   |                    |                                                                        |
| (III) bromide             | SbBr <sub>3</sub>                               | 361.47      | 4.35                              | 96.6                   | 280                | s acet, bz, chl                                                        |
| (III) chloride            | SbCl <sub>3</sub>                               | 228.12      | 3.14 <sup>20</sup>                | 73.4                   | 220.3              | 10 g/100 mL <sup>20</sup> aq; s alc, bz, chl                           |
| (V) chloride              | SbCl <sub>5</sub>                               | 299.02      | 2.336 <sup>20</sup>               | 3.5                    | 79 <sup>22mm</sup> | d aq; s HCl, chl, CCl <sub>4</sub>                                     |
| (III) fluoride            | SbF <sub>3</sub>                                | 178.75      | 4.379 <sup>20</sup>               | 292                    | 376                | 444 g/100 mL <sup>20</sup> aq                                          |
| (V) fluoride              | SbF <sub>5</sub>                                | 216.75      | 2.99 <sup>23</sup>                | 8.3                    | 141                | d viol aq; s HOAc; forms solids<br>with alc, bz, CS <sub>2</sub> , eth |
| hydride (stibine)         | SbH <sub>3</sub>                                | 124.78      | 5.475 g/L                         | –91.5                  | –18.4              | 20 mL/100 mL <sup>20</sup> aq; s CS <sub>2</sub> , alc                 |
| (III) iodide              | SbI <sub>3</sub>                                | 502.47      | 4.92                              | 168                    | 401                | g/100 g <sup>25</sup> : 1.16 bz, 1.24 tol, 0.16 chl                    |
| (III) oxide (valentinite) | Sb <sub>2</sub> O <sub>3</sub>                  | 291.52      | 5.7                               | 655                    | 1425               | v sl s aq; s HCl, KOH                                                  |
| (V) oxide                 | Sb <sub>2</sub> O <sub>3</sub>                  | 323.52      | 3.78                              | –O <sub>2</sub> , >300 |                    | v sl s aq; sl s warm KOH, eth                                          |
| (III) selenide            | Sb <sub>2</sub> Se <sub>3</sub>                 | 480.40      | 5.81                              | 612                    |                    | v sl s aq; s conc HCl                                                  |
| (III) sulfate             | Sb <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> | 531.71      | 3.62                              | d                      |                    | sl s aq                                                                |
| (III) sulfide             | Sb <sub>2</sub> S <sub>3</sub>                  | 339.72      | 4.56                              | 546                    |                    | 0.002 <sup>20</sup> aq (d); s H <sub>2</sub> SO <sub>4</sub>           |
| (V) sulfide               | Sb <sub>2</sub> S <sub>5</sub>                  | 403.85      | 4.120                             | 75 d                   |                    | i aq; s HCl (d), NaOH                                                  |
| (III) telluride           | Sb <sub>2</sub> Te <sub>3</sub>                 | 626.32      | 6.52                              | 620                    |                    | i aq; s HNO <sub>3</sub>                                               |
| triethyl                  | Sb(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> | 209.0       | 1.324 <sup>14</sup>               | –29                    | 159.5              | i aq                                                                   |
| trimethyl                 | Sb(CH <sub>3</sub> ) <sub>3</sub>               | 166.9       | 1.523 <sup>15</sup>               |                        | 80.6               | sl s aq                                                                |
| Argon                     | Ar                                              | 39.948(1)   | 1.7824 g/L <sup>0</sup>           | –189.38                | –185.87            | 3.36 mL/100 mL <sup>20</sup> aq                                        |
| Arsenic                   | As                                              | 74.92159(2) | 5.727 <sup>25</sup> <sub>4</sub>  | 817                    | subl 615           | i aq; s HNO <sub>3</sub>                                               |
| (III) bromide             | AsBr <sub>3</sub>                               | 314.63      | 3.3972 <sup>25</sup> <sub>4</sub> | 31.1                   | 220.0              | hyd aq; s HCl, CS <sub>2</sub> , PE                                    |
| (III) chloride            | AsCl <sub>3</sub>                               | 181.28      | 2.1497 <sup>25</sup> <sub>5</sub> | –16.2                  | 130.2              | misc chl, CCl <sub>4</sub> , eth; s HCl                                |
| (di-) disulfide           | As <sub>2</sub> S <sub>2</sub>                  | 213.97      | 3.254 <sup>19</sup>               | 320                    | 565                | s alkali; v sl s bz                                                    |
| (III) fluoride            | AsF <sub>3</sub>                                | 131.92      | 2.73 <sup>15</sup> <sub>3</sub>   | –5.95                  | 57.8               | s alc, bz, eth, HF                                                     |
| (V) fluoride              | AsF <sub>5</sub>                                | 169.91      | 7.46 g/L                          | –79.8                  | –52.8              | hyd aq; s alc, bz, eth                                                 |
| (III) hydride (arsine)    | AsH <sub>3</sub>                                | 77.95       | 3.420 g/L                         | –116.9                 | –62.5              | 28 mL/100 mL <sup>20</sup> aq; s bz, chl                               |
| (III) iodide              | AsI <sub>3</sub>                                | 455.63      | 4.73                              | 140.9                  | 424                | s bz, tol; sl s aq, alc, eth                                           |
| (III) oxide (arsenolite)  | As <sub>2</sub> O <sub>3</sub>                  | 197.84      | 3.86                              | 274                    | 460                | 1.8 <sup>20</sup> aq; s alc                                            |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

|             | Name                         | Formula                                                                           | Formula weight | Density             | Melting point,                     | Boiling point,         | Solubility in<br>100 parts solvent                               |
|-------------|------------------------------|-----------------------------------------------------------------------------------|----------------|---------------------|------------------------------------|------------------------|------------------------------------------------------------------|
|             |                              |                                                                                   |                |                     | °C                                 | °C                     |                                                                  |
| <b>3.18</b> | Arsenic ( <i>continued</i> ) |                                                                                   |                |                     |                                    |                        |                                                                  |
|             | (III) oxide (claudeite)      | As <sub>2</sub> O <sub>3</sub>                                                    | 197.84         | 3.74                | 313                                | 460                    | sl s aq; s dil acid, alk                                         |
|             | (V) oxide                    | As <sub>2</sub> O <sub>5</sub>                                                    | 229.84         | 4.32                | 315                                | d 800                  | 66 g/100 mL <sup>20</sup> aq; s alc                              |
|             | (III) selenide               | As <sub>2</sub> Se <sub>3</sub>                                                   | 386.72         | 4.75                | 260                                |                        | s alkali, HNO <sub>3</sub>                                       |
|             | (III) sulfide                | As <sub>2</sub> S <sub>3</sub>                                                    | 246.04         | 3.460               | 310                                | 707                    | i aq; s alk, slowly s hot HCl                                    |
|             | (V) sulfide                  | As <sub>2</sub> S <sub>5</sub>                                                    | 310.17         |                     | subl 500                           |                        | 0.0003 aq; s alkali, HNO <sub>3</sub>                            |
|             | (III) telluride              | As <sub>2</sub> Te <sub>3</sub>                                                   | 532.64         | 6.50                | 621                                |                        |                                                                  |
|             | Astatine                     | At                                                                                | 210            |                     | 302                                |                        |                                                                  |
|             | Barium                       | Ba                                                                                | 137.33         | 3.51 <sup>20</sup>  | 726.9                              | 1845                   | d aq to Ba(OH)                                                   |
|             | acetate hydrate              | Ba(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O | 273.43         | 2.19                | anhyd 110                          | d 150                  | 58.8 g/100 mL <sup>0</sup> aq; 0.014 alc                         |
|             | benzenesulfonate             | Ba(O <sub>3</sub> SC <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>                   | 451.70         |                     |                                    |                        | s aq; sl s alc                                                   |
|             | bromate hydrate              | Ba(BrO <sub>3</sub> ) <sub>2</sub> · H <sub>2</sub> O                             | 411.14         | 3.99 <sup>18</sup>  | d 260                              |                        | 0.96 <sup>30</sup> aq; s acet; i alc                             |
|             | bromide                      | BaBr <sub>2</sub>                                                                 | 297.14         | 4.781               | 856                                | 1835                   | 92 g/100 mL <sup>0</sup> aq; s MeOH, acet                        |
|             | carbonate                    | BaCO <sub>3</sub>                                                                 | 197.34         | 4.2865              | d 1300 to BaO<br>+ CO <sub>2</sub> |                        | 0.0024 aq; s acids                                               |
|             | chlorate hydrate             | Ba(ClO <sub>3</sub> ) <sub>2</sub> · H <sub>2</sub> O                             | 322.24         | 3.179               | anhyd 120                          | – O <sub>2</sub> , 250 | 34 g/100 mL <sup>20</sup> aq; sl s alc, acet                     |
|             | chloride                     | BaCl <sub>2</sub>                                                                 | 208.24         | 3.856 <sup>24</sup> | 962                                | 1560                   | 36 g/100 mL <sup>20</sup> aq; s MeOH; i acet,<br>EtAc            |
|             | chloride dihydrate           | BaCl <sub>2</sub> · 2H <sub>2</sub> O                                             | 244.26         | 3.097               | anhyd 113                          |                        | 31.7 g/100 mL <sup>0</sup> aq                                    |
|             | chromate(VI)                 | BaCrO <sub>4</sub>                                                                | 253.33         | 4.498 <sup>20</sup> | d                                  |                        | 0.001 <sup>20</sup> aq; s mineral acids                          |
|             | cyanide                      | Ba(CN) <sub>2</sub>                                                               | 189.36         |                     |                                    |                        | 80 g/100 mL <sup>14</sup> aq; s alc                              |
|             | fluoride                     | BaF <sub>2</sub>                                                                  | 175.32         | 4.89                | 1368                               | 2260                   | 0.161 <sup>20</sup> aq; s acids                                  |
|             | hexafluorosilicate           | Ba[SiF <sub>6</sub> ]                                                             | 279.40         | 4.29 <sup>21</sup>  | d 300                              |                        | 0.0235 <sup>25</sup> aq; s NH <sub>4</sub> Cl soln; i alc        |
|             | hydrogen phosphate           | BaHPO <sub>4</sub>                                                                | 233.31         | 4.165 <sup>15</sup> | d 410                              |                        | 0.01 aq; s HCl, HNO <sub>3</sub>                                 |
|             | hydroxide 8-water            | Ba(OH) <sub>2</sub> · 8H <sub>2</sub> O                                           | 315.48         | 2.18 <sup>16</sup>  | 78                                 |                        | 3.9 <sup>20</sup> aq                                             |
|             | iodate                       | Ba(IO <sub>3</sub> ) <sub>2</sub>                                                 | 487.13         | 5.23 <sup>20</sup>  | d 476                              |                        | 0.033 <sup>20</sup> aq; s HCl                                    |
|             | iodide                       | BaI <sub>2</sub>                                                                  | 391.14         | 5.15                | 711                                | 2027                   | 169 g/100 mL <sup>20</sup> aq; s alc, acet                       |
|             | manganate(VI)(2–)            | BaMnO <sub>4</sub>                                                                | 256.26         | 4.85                |                                    |                        | disprop to Ba(MnO <sub>4</sub> ) <sub>2</sub> + MnO <sub>2</sub> |
|             | molybdate                    | BaMoO <sub>4</sub>                                                                | 297.27         | 4.975               | 1450                               |                        | 0.0058 <sup>25</sup> aq                                          |
|             | niobate                      | Ba(NbO <sub>3</sub> ) <sub>2</sub>                                                | 419.14         | 5.44                | 1455                               |                        | i aq                                                             |
|             | nitrate                      | Ba(NO <sub>3</sub> ) <sub>2</sub>                                                 | 261.34         | 3.24 <sup>23</sup>  | 592                                | d                      | 5.0 aq; v sl s alc, acet                                         |
|             | nitrite hydrate              | Ba(NO <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O                              | 247.35         | 3.173 <sup>30</sup> | d 115                              |                        | 54.8 g/100 mL <sup>0</sup> aq; i alc                             |

|                                 |                                                                  |        |                      |                        |                          |                                                                    |
|---------------------------------|------------------------------------------------------------------|--------|----------------------|------------------------|--------------------------|--------------------------------------------------------------------|
| oxalate                         | BaC <sub>2</sub> O <sub>4</sub>                                  | 225.35 | 2.658                | 400 d                  |                          | i aq                                                               |
| oxide                           | BaO                                                              | 153.33 | 5.72                 | 1973                   | 3088                     | 3.5 <sup>20</sup> aq; s acids, EtOH                                |
| perchlorate                     | Ba(ClO <sub>4</sub> ) <sub>2</sub>                               | 336.23 | 3.20                 | 505                    |                          | g/100 mL <sup>25</sup> ; 129 aq, 78 EtOH, 42 BuOH, 81 EtOAc; i eth |
| perchlorate 3-water             | Ba(ClO <sub>4</sub> ) <sub>2</sub> · 3H <sub>2</sub> O           | 390.27 | 2.74                 | d 400                  |                          | 198 g/100 mL <sup>25</sup> aq; s MeOH; sl s acet                   |
| permanganate                    | Ba(MnO <sub>4</sub> ) <sub>2</sub>                               | 375.20 | 3.77                 | d 200                  |                          | v s aq                                                             |
| peroxide                        | BaO <sub>2</sub>                                                 | 169.33 | 4.96                 | 450 d                  | – O <sub>2</sub> , 800   | 1.5 <sup>9</sup> aq                                                |
| selenide                        | BaSe                                                             | 216.29 | 5.02                 | 1780                   |                          | d aq                                                               |
| stearate                        | Ba(C <sub>18</sub> H <sub>35</sub> O <sub>2</sub> ) <sub>2</sub> | 704.28 | 1.145                | 160                    |                          | i aq                                                               |
| sulfate                         | BaSO <sub>4</sub>                                                | 233.39 | 4.50 <sup>15</sup>   | 1580                   | d > 1600                 | 0.00285 aq                                                         |
| sulfide                         | BaS                                                              | 169.39 | 4.25 <sup>15</sup>   | 2230                   |                          | 7.9 <sup>20</sup> aq; dec in acids                                 |
| sulfite                         | BaSO <sub>3</sub>                                                | 217.39 | 4.44                 | d                      |                          | 0.02 <sup>9</sup> aq; i alc                                        |
| tetracyanoplatinate(II)-4-water | Ba[Pt(CN) <sub>4</sub> ] · 4H <sub>2</sub> O                     | 508.54 | 2.076                |                        |                          | 2.86 aq; i alc                                                     |
| thiocyanate 2-water             | Ba(SCN) <sub>2</sub> · 2H <sub>2</sub> O                         | 289.53 | 2.286 <sup>18</sup>  | d 160                  |                          | 170 g/100 mL <sup>20</sup> aq; s alc, acet                         |
| thiosulfate hydrate             | BaS <sub>2</sub> O <sub>3</sub> · H <sub>2</sub> O               | 267.47 | 3.5 <sup>18</sup>    | d 220                  |                          | 0.21 <sup>20</sup> aq; i alc, acet, eth, CS                        |
| titanate(IV)(2–)                | BaTiO <sub>3</sub>                                               | 233.19 | 6.02                 | 1625                   |                          | i aq                                                               |
| vanadate                        | Ba <sub>3</sub> (VO <sub>4</sub> ) <sub>2</sub>                  | 641.86 | 5.14                 | 707                    |                          |                                                                    |
| zirconate                       | BaZrO <sub>3</sub>                                               | 276.55 | 5.52                 | 2500                   |                          | i aq, alk; sl s acids                                              |
| Berkelium (α form)              | Bk                                                               | 247    | 14.78                | 1050                   |                          |                                                                    |
| (β form)                        | Bk                                                               | 247    | 13.25                | 986                    |                          |                                                                    |
| Beryllium                       | Be                                                               | 9.012  | 1.8477 <sup>20</sup> | 1287                   | 2467                     | i aq; s acid, alk                                                  |
| bromide                         | BeBr <sub>2</sub>                                                | 168.82 | 3.465 <sup>25</sup>  | 508                    | 521                      | v s aq; s alc; 18.6 pyr                                            |
| carbide                         | Be <sub>2</sub> C                                                | 30.04  | 1.90 <sup>15</sup>   | d > 2127               |                          | d aq; s acids, alkali giving CH <sub>4</sub>                       |
| chloride                        | BeCl <sub>2</sub>                                                | 79.92  | 1.899 <sup>25</sup>  | 415 (alpha)            | 482.3                    | 42 g/100 mL aq; s alc, eth, pyr, CS <sub>2</sub>                   |
| fluoride                        | BeF <sub>2</sub>                                                 | 47.01  | 1.986                | 555                    | subl 1036 <sup>1mm</sup> | v s aq (slowly)                                                    |
| hydride                         | BeH <sub>2</sub>                                                 | 11.03  | 0.65                 | – H <sub>2</sub> , 220 |                          | d aq (slowly), acids (rapidly)                                     |
| hydroxide                       | Be(OH) <sub>2</sub>                                              | 43.03  | 1.909                | 93                     |                          | s hot conc acids and alkali (viol)                                 |
| iodide                          | BeI <sub>2</sub>                                                 | 262.82 | 4.32                 | 480                    | 487                      | hyd aq violently; s alc, eth, CS <sub>2</sub>                      |
| nitrate 3-water                 | Be(NO <sub>3</sub> ) <sub>2</sub> · 3H <sub>2</sub> O            | 187.07 | 1.557                | 60.5                   | d 125                    | 166 g/100 mL <sup>20</sup> aq                                      |
| nitride                         | Be <sub>3</sub> N <sub>2</sub>                                   | 55.05  | 2.71                 | 2200                   |                          | d hot aq, alkali                                                   |
| oxide                           | BeO                                                              | 25.01  | 3.025                | 2578 (alpha)           | 3787                     | s conc H <sub>2</sub> SO <sub>4</sub>                              |
| selenate 4-water                | BeSeO <sub>4</sub> · 4H <sub>2</sub> O                           | 224.03 | 2.03                 | anhyd 300              | d 560                    | 49 g/100 mL <sup>25</sup> aq                                       |
| silicate                        | Be <sub>2</sub> SiO <sub>4</sub>                                 | 110.11 | 3.0                  | 1560                   |                          | i aq                                                               |
| sulfate 4-water                 | BeSO <sub>4</sub> · 4H <sub>2</sub> O                            | 177.14 | 1.713                | anhyd 270              | d 580                    | 39 g/100 mL <sup>20</sup> aq; i alc                                |
| sulfide                         | BeS                                                              | 41.08  | 2.36                 | d                      |                          | i aq; s HNO <sub>3</sub>                                           |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                                      | Formula                                               | Formula weight | Density                | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                 |
|-------------------------------------------|-------------------------------------------------------|----------------|------------------------|----------------------|----------------------|--------------------------------------------------------------------|
| Bismuth                                   | Bi                                                    | 208.9804       | 9.78                   | 271.5                | 1564                 | i aq; s hot H <sub>2</sub> SO <sub>4</sub>                         |
| (III) bromide                             | BiBr <sub>3</sub>                                     | 448.69         | 5.72                   | 218                  | 453                  | d aq; s dil acids, acet                                            |
| bromide oxide                             | BiBrO                                                 | 304.88         | 8.08 <sup>215</sup>    | d                    |                      | i aq; s acids                                                      |
| (III) chloride                            | BiCl <sub>3</sub>                                     | 315.34         | 4.75                   | 233.5                | 447                  | d aq; s HCl, alc, eth, acet                                        |
| chloride oxide                            | BiClO                                                 | 260.43         | 7.72 <sup>15</sup>     | d                    |                      | i aq; s HCl                                                        |
| (III) fluoride                            | BiF <sub>3</sub>                                      | 265.98         | 8.32                   | 727                  | 900                  | i aq; s HF                                                         |
| (V) fluoride                              | BiF <sub>5</sub>                                      | 303.97         | 5.55 <sup>25</sup>     | 154.4                | subl 550             | d (viol) aq giving O <sub>3</sub> + BiF <sub>3</sub>               |
| hydride                                   | BiH <sub>3</sub>                                      | 212.00         | 9.303 g/L              | − 67                 | 16.8                 | very unstable liquid                                               |
| (III) hydroxide                           | Bi(OH) <sub>3</sub>                                   | 260.00         | 4.962 <sup>15</sup>    | − water, 100         |                      | d aq; s HCl                                                        |
| (III) iodide                              | BiI <sub>3</sub>                                      | 589.69         | 5.778 <sup>20</sup>    | 408.6                | subl 439             | i aq; s HCl, alc                                                   |
| iodide oxide                              | BiIO                                                  | 351.88         | 7.922                  | d red heat           |                      | i aq; s HCl                                                        |
| (III) nitrate 5-water                     | Bi(NO <sub>3</sub> ) <sub>3</sub> · 5H <sub>2</sub> O | 485.07         | 2.83                   | anhyd 80             |                      | d aq; s HNO <sub>3</sub> , acet, glyc                              |
| (III) oxide                               | Bi <sub>2</sub> O <sub>3</sub>                        | 465.96         | 8.76                   | 817                  | 1890                 | i aq; s HCl, HNO <sub>3</sub>                                      |
| (V) oxide                                 | Bi <sub>2</sub> O <sub>5</sub>                        | 497.96         | 5.10                   | d 150                |                      | i aq; s KOH                                                        |
| (III) phosphate                           | BiPO <sub>4</sub>                                     | 303.95         | 6.323 <sup>15</sup>    | d                    |                      | s conc HCl, HNO <sub>3</sub>                                       |
| (III) selenide                            | Bi <sub>2</sub> Se <sub>3</sub>                       | 654.84         | 7.70 <sup>20</sup>     | 710 d                | d                    | i aq; d aq reg                                                     |
| (III) sulfate                             | Bi <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>       | 706.14         | 5.08                   | d 405                |                      | d aq, alc; s HCl                                                   |
| (III) sulfide                             | Bi <sub>2</sub> S <sub>3</sub>                        | 514.16         | 6.78                   | 850                  |                      | i aq, EtAc; s HNO <sub>3</sub> , HCl                               |
| (III) telluride                           | Bi <sub>2</sub> Te <sub>3</sub>                       | 800.76         | 7.74                   | 588.5                |                      | i aq; s alc                                                        |
| Boranes                                   |                                                       |                |                        |                      |                      |                                                                    |
| diborane(6)                               | B <sub>2</sub> H <sub>6</sub>                         | 27.67          | 1.214 g/L              | − 165.5              | − 92.5               | FP − 68; s NH <sub>4</sub> OH, conc H <sub>2</sub> SO <sub>4</sub> |
| tetraborane(10)                           | B <sub>4</sub> H <sub>10</sub>                        | 53.32          | 2.340 g/L              | − 120                | 18                   | sl s aq; s bz                                                      |
| pentaborane(9)                            | B <sub>5</sub> H <sub>9</sub>                         | 63.13          | 0.60                   | − 46.81              | 60.0                 | hyd aq                                                             |
| pentaborane(11)                           | B <sub>5</sub> H <sub>11</sub>                        | 65.14          | 0.745                  | − 123                | 63                   | d aq                                                               |
| hexaborane(10)                            | B <sub>6</sub> H <sub>10</sub>                        | 74.95          | 0.67                   | − 62.3               | 108 d                | d hot aq                                                           |
| decaborane(14)                            | B <sub>10</sub> H <sub>14</sub>                       | 122.22         | 0.948                  | 99.5                 | 213                  | sl s aq; s bz, CS <sub>2</sub> , eth                               |
| Borazine                                  | B <sub>3</sub> H <sub>6</sub> N <sub>3</sub>          | 80.50          | lq: 0.81 <sup>bp</sup> | − 58                 | 55                   | sl s aq (d)                                                        |
| Boric acids, <i>see</i> under<br>Hydrogen |                                                       |                |                        |                      |                      |                                                                    |
| Boron                                     | B                                                     | 10.811         | 2.34                   | 2076                 | 3864                 | i aq                                                               |
| carbide                                   | B <sub>4</sub> C                                      | 55.25          | 2.510 <sup>25</sup>    | 2350                 | >3500                | s fused alkalis                                                    |
| tribromide                                | BBr <sub>3</sub>                                      | 250.52         | 2.6                    | − 46.0               | 91.3                 | d aq, alc                                                          |

|                             |                                                       |           |                                   |                              |                    |                                                         |
|-----------------------------|-------------------------------------------------------|-----------|-----------------------------------|------------------------------|--------------------|---------------------------------------------------------|
| trichloride                 | $\text{BCl}_3$                                        | 117.17    | 5.141 g/L                         | − 107                        | 12.7               | d aq, alc                                               |
| trifluoride                 | $\text{BF}_3$                                         | 67.81     | 3.077 g/L <sup>STP</sup>          | − 127.1                      | − 100.4            | 332 g/100 mL <sup>0</sup> aq; s bz, chl, $\text{CCl}_4$ |
| trifluoride 1-diethyl ether | $\text{BF}_3 \cdot \text{O}(\text{C}_2\text{H}_5)_2$  | 141.94    | 1.125                             | − 60.4                       | 125.7              | d aq                                                    |
| trifluoride 1-methanol      | $\text{BF}_3 \cdot \text{HOCH}_3$                     | 131.89    | 1.203                             |                              | 59 <sup>4mm</sup>  |                                                         |
| nitride                     | $\text{BN}$                                           | 24.82     | 2.18                              | 2967                         |                    | sl s hot acids                                          |
| oxide                       | $\text{B}_2\text{O}_3$                                | 69.62     | 2.55                              | 450.0                        | 2065               | 3.3 aq (slowly); s alc, glyc                            |
| Bromine                     | $\text{Br}_2$                                         | 159.808   | 3.1023 <sup>25</sup> <sub>4</sub> | − 7.25                       | 58.8               | 3.4 g/100 mL <sup>20</sup> aq; v s alc, chl, eth        |
| pentafluoride               | $\text{BF}_5$                                         | 174.90    | 2.460                             | − 60.5                       | 40.76              | explodes with water; s HF                               |
| trifluoride                 | $\text{BF}_3$                                         | 136.90    | 2.803 <sup>25</sup>               | 8.77                         | 125.74             | d viol aq; d alk; smokes in air                         |
| Cadmium                     | $\text{Cd}$                                           | 112.411   | 8.65 <sup>25</sup>                | 321                          | 765                | i aq, alk; s $\text{HNO}_3$ , hot HCl                   |
| acetate                     | $\text{Cd}(\text{C}_2\text{H}_3\text{O}_2)_2$         | 230.50    | 2.341                             | 255                          | d                  | v s aq; s alc                                           |
| bromide                     | $\text{CdBr}_2$                                       | 272.22    | 5.192                             | 566                          | 963                | 99 g/100 mL <sup>20</sup> aq; s acet; sl s eth          |
| carbonate                   | $\text{CdCO}_3$                                       | 172.42    | 4.258 <sup>4</sup>                | d 500                        |                    | s acids, $\text{NH}_4\text{OH}$                         |
| chloride                    | $\text{CdCl}_2$                                       | 183.32    | 4.05 <sup>25</sup>                | 568                          | 960                | 120 g/100 mL <sup>25</sup> aq                           |
| cyanide                     | $\text{Cd}(\text{CN})_2$                              | 164.44    | 2.226                             | d 200                        |                    | 1.71 g/100 mL <sup>15</sup> aq; sl s alc                |
| fluoride                    | $\text{CdF}_2$                                        | 150.41    | 6.33                              | 1110                         | 1748               | 4.3 g/100 mL <sup>25</sup> aq                           |
| hydroxide                   | $\text{Cd}(\text{OH})_2$                              | 146.43    | 4.79                              | − $\text{H}_2\text{O}$ , 130 | $\text{CaO}$ , 200 | 0.00026 <sup>20</sup> aq; s acids                       |
| iodide                      | $\text{CdI}_2$                                        | 366.22    | 5.670                             | 388                          | 742                | 84.7 g/100 mL <sup>20</sup> aq; s alc, acet, eth        |
| nitrate 4-water             | $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  | 308.48    | 2.455                             | 59.4                         |                    | 167 g/100 mL <sup>25</sup> aq; s alc, acet              |
| oxide                       | $\text{CdO}$                                          | 128.41    | 8.15 cubic                        | 1540                         |                    | i aq; s acids                                           |
| phosphide                   | $\text{Cd}_3\text{P}_2$                               | 399.18    | 5.96                              | 700                          |                    | s dil acid                                              |
| selenide                    | $\text{CdSe}$                                         | 191.37    | 5.81 <sup>15</sup>                | 1350                         |                    | i aq; d acids                                           |
| sulfate-water (3/8)         | $3\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$            | 769.56    | 3.08                              | monohydrate, 80              |                    | 94.4 g/100 mL <sup>25</sup> aq; i alc, EtAc             |
| sulfide                     | $\text{CdS}$                                          | 144.48    | 4.83                              | 1750                         |                    | 0.13 <sup>18</sup> aq; s acids                          |
| telluride                   | $\text{CdTe}$                                         | 240.01    | 6.20 <sup>15</sup> <sub>4</sub>   | 1041                         |                    | i aq; d $\text{HNO}_3$                                  |
| tungstate(VI)               | $\text{CdWO}_4$                                       | 360.25    | 8.0                               |                              |                    | i aq, dil acids; s alkali CN's                          |
| Calcium                     | $\text{Ca}$                                           | 40.078(4) | 1.55                              | 842                          | 1484               | d aq; s acids                                           |
| acetate                     | $\text{Ca}(\text{C}_2\text{H}_3\text{O}_2)_2$         | 158.17    | 1.50                              | d > 160                      |                    | 37.4 g/100 mL <sup>0</sup> aq; i alc, bz, acet          |
| arsenate                    | $\text{Ca}_3(\text{AsO}_4)_2$                         | 398.07    | 3.620                             |                              |                    | 0.013 <sup>25</sup> aq                                  |
| bromide                     | $\text{CaBr}_2$                                       | 199.89    | 3.38                              | 742                          | 1815               | 143 g/100 mL <sup>20</sup> aq; v s alc, acet            |
| carbide                     | $\text{CaC}_2$                                        | 64.10     | 2.222                             | 2300                         |                    | reacts with aq giving $\text{C}_2\text{H}_2$            |
| carbonate (aragonite)       | $\text{CaCO}_3$                                       | 100.09    | 2.83                              | d 825 to $\text{CaO}$        |                    | s dil acids                                             |
| carbonate (calcite)         | $\text{CaCO}_3$                                       | 100.09    | 2.711                             | d 825 to $\text{CaO}$        |                    | 0.0013 g/100 mL <sup>20</sup> ; s acids                 |
| chlorate 2-water            | $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$ | 243.01    | 2.711                             | anhyd 100                    |                    | 167 g/100 mL <sup>20</sup> aq; s alc                    |
| chloride                    | $\text{CaCl}_2$                                       | 110.98    | 2.16 <sup>3</sup> <sub>4</sub>    | 775                          | ca. 1940           | 42 g/100 mL <sup>20</sup> aq; s alc, acet               |
| chloride 6-water            | $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$             | 219.07    | 1.71                              | anhyd 200                    |                    | 74.5 g/100 mL <sup>20</sup> aq; v s alc                 |
| chlorite                    | $\text{Ca}(\text{ClO}_2)_2$                           | 174.99    | 2.71 <sup>25</sup>                | 100                          |                    | 167 g/100 mL aq; s alc                                  |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                         | Formula                                                                            | Formula weight | Density             | Melting point,<br>°C     | Boiling point,<br>°C | Solubility in<br>100 parts solvent                 |
|------------------------------|------------------------------------------------------------------------------------|----------------|---------------------|--------------------------|----------------------|----------------------------------------------------|
| Calcium ( <i>continued</i> ) |                                                                                    |                |                     |                          |                      |                                                    |
| chromate(VI) 2-water         | CaCrO <sub>4</sub> · 2H <sub>2</sub> O                                             | 192.10         | 2.50                | anhyd 200                |                      | sl s aq; s dil acids                               |
| citrate 4-water              | CaC <sub>6</sub> H <sub>6</sub> O <sub>7</sub> · 4H <sub>2</sub> O                 | 570.51         |                     | anhyd 120                |                      | 0.10 aq; i alc                                     |
| cyanamide                    | CaCN <sub>2</sub>                                                                  | 80.10          | 2.29                | ca. 1340                 | subl                 | no known solv without dec                          |
| cyanide                      | Ca(CN) <sub>2</sub>                                                                | 92.11          |                     | s > 350                  |                      | s aq                                               |
| dichromate(VI)               | CaCr <sub>2</sub> O <sub>7</sub>                                                   | 256.10         | 2.370 <sup>30</sup> | d > 100                  |                      | v s aq; i eth; d alc                               |
| dihydrogen phosphate         | Ca(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> · H <sub>2</sub> O                | 252.07         | 2.220 <sup>18</sup> | anhyd 100                | d 200                | 1.8 <sup>30</sup> aq                               |
| hydrate                      |                                                                                    |                |                     |                          |                      |                                                    |
| diphosphate (pyrophosphate)  | Ca <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                                      | 254.10         | 3.09                | 1353                     |                      | i aq; s HCl, HNO <sub>3</sub>                      |
| fluoride                     | CaF <sub>2</sub>                                                                   | 78.08          | 3.180               | 1418                     | 2533                 | 0.0015 <sup>20</sup> aq; s conc mineral acids      |
| formate                      | Ca(CHO <sub>2</sub> ) <sub>2</sub>                                                 | 130.11         | 2.015               | 300 d                    |                      | 16.6 g/100 mL <sup>20</sup> aq; i alc              |
| (+)gluconate                 | Ca[OOC(CHOH) <sub>2</sub> CH <sub>4</sub> OH] <sub>2</sub>                         | 430.38         |                     |                          |                      | 3.72 <sup>20</sup> aq                              |
| glycerophosphate             | Ca[C <sub>3</sub> H <sub>5</sub> (OH) <sub>3</sub> ]PO <sub>4</sub>                | 210.16         |                     | d > 170                  |                      | 1.66 <sup>20</sup> aq; i alc                       |
| hexafluorosilicate           | Ca[SiF <sub>6</sub> ]                                                              | 182.17         | 2.662               |                          |                      | i aq, acet                                         |
| hydride                      | CaH <sub>2</sub>                                                                   | 42.09          | 1.70                | 1000                     |                      | d aq, alc                                          |
| hydroxide                    | Ca(OH) <sub>2</sub>                                                                | 74.09          | 2.343               | – H <sub>2</sub> O, 580  |                      | 0.17 <sup>10</sup> aq; s acids                     |
| hypochlorite                 | Ca(OCl) <sub>2</sub>                                                               | 142.99         | 2.35                | 100 d                    |                      | d aq evolving Cl <sub>2</sub> ; i alc              |
| iodate                       | Ca(IO <sub>3</sub> ) <sub>2</sub>                                                  | 389.88         | 4.519 <sup>15</sup> | d > 540                  |                      | 0.10 <sup>0</sup> aq; i alc                        |
| iodide                       | CaI <sub>2</sub>                                                                   | 293.89         | 3.956               | 783                      | 1755                 | 68 g/100 mL <sup>20</sup> aq; v s alc, acet; i eth |
| lactate 5-water              | Ca(C <sub>3</sub> H <sub>5</sub> O <sub>3</sub> ) <sub>2</sub> · 5H <sub>2</sub> O | 308.30         |                     | – 3H <sub>2</sub> O, 100 | anhyd 120            | 5.4 <sup>15</sup> aq; v sl s alc                   |
| magnesium carbonate          | Ca[Mg(CO <sub>3</sub> ) <sub>2</sub> ]                                             | 184.41         | 2.872               | d 730                    |                      | 0.032 <sup>18</sup> aq; s HCl                      |
| molybdate(VI)(2–)            | CaMoO <sub>4</sub>                                                                 | 200.02         | 4.35                |                          |                      | s conc mineral acids                               |
| nitrate                      | Ca(NO <sub>3</sub> ) <sub>2</sub>                                                  | 164.09         | 2.504               | 56l                      |                      | 152 g/100 mL <sup>30</sup> aq                      |
| nitride                      | Ca <sub>3</sub> N <sub>2</sub>                                                     | 148.25         | 2.67                | 1195                     |                      | d aq; s dilute acids (d)                           |
| nitrite 4-water              | Ca(NO <sub>2</sub> ) <sub>2</sub> · 4H <sub>2</sub> O                              | 204.15         | 1.674               | d                        |                      | 84.5 g/100 mL <sup>18</sup> aq; sl s alc           |
| oleate                       | Ca(C <sub>18</sub> H <sub>33</sub> O <sub>2</sub> ) <sub>2</sub>                   | 603.01         |                     | 83–84                    | d > 400              | 0.04 aq; s chl, bz; v sl s alc, eth                |
| oxalate hydrate              | CaC <sub>2</sub> O <sub>4</sub> · H <sub>2</sub> O                                 | 146.11         | 2.2                 | anhyd 200                |                      | 0.0006 aq; s acids                                 |
| oxide                        | CaO                                                                                | 56.08          | 3.34                | 2900                     | 3500                 | 0.13 <sup>25</sup> aq; s acids                     |
| palmitate                    | Ca(C <sub>16</sub> H <sub>31</sub> O <sub>2</sub> ) <sub>2</sub>                   | 550.93         |                     | d > 155                  |                      | 0.003 aq; sl s bz, chl, HOAc                       |
| (+)panthothenate             | Ca[O <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NHO-                             | 476.55         |                     | d 195–196                |                      | 36 g/100 mL aq; sl s alc, acet                     |
| (vitamin B <sub>3</sub> )    | CH(OH)C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> OH] <sub>2</sub>            |                |                     |                          |                      |                                                    |



|                        |                                                                         |        |                                                     |                             |           |                                                                        |
|------------------------|-------------------------------------------------------------------------|--------|-----------------------------------------------------|-----------------------------|-----------|------------------------------------------------------------------------|
| perchlorate            | $\text{Ca}(\text{ClO}_4)_2$                                             | 238.98 | 2.65                                                | d 270                       |           | g/100 mL <sup>25</sup> : 112 aq, 89.5 EtOH, 68 BuOH, 57 EtOAc, 43 acet |
| permanganate 5-water   | $\text{Ca}(\text{MnO}_4)_2 \cdot 5\text{H}_2\text{O}$                   | 368.03 | 2.4                                                 | d                           |           | 338 g/100 mL aq                                                        |
| peroxide               | $\text{CaO}_2$                                                          | 72.08  | 2.92                                                | explodes 275                |           | sl s aq; s acids                                                       |
| phenoxide              | $\text{Ca}(\text{OC}_6\text{H}_5)_2$                                    | 226.28 | d in air                                            |                             |           | sl s aq, alc                                                           |
| phosphate              | $\text{Ca}_3(\text{PO}_4)_2$                                            | 310.18 | 3.14                                                | 1670                        |           | 0.03 <sup>25</sup> aq; s HCl, HNO <sub>3</sub> ; i alc                 |
| phosphide              | $\text{Ca}_3\text{P}_2$                                                 | 182.18 | 2.51                                                | ca. 1600                    |           | d aq; s acids; i alc, eth                                              |
| phosphinate            | $\text{Ca}(\text{PH}_2\text{O}_2)_2$                                    | 170.06 |                                                     | d > 300                     |           | 15.4 g/100 mL aq; sl s glyc                                            |
| propanoate             | $\text{Ca}(\text{OOCCH}_3\text{H}_5)_2$                                 | 186.22 |                                                     |                             |           | s aq; sl s alc; i acet, bz                                             |
| salicylate 2-water     | $\text{Ca}(\text{C}_7\text{H}_5\text{O}_3)_2 \cdot 2\text{H}_2\text{O}$ | 350.34 |                                                     | anhyd 200                   | d 240     | 2.8 <sup>15</sup> aq; 0.015 <sup>16</sup> EtOH                         |
| selenate 2-water       | $\text{CaSeO}_4 \cdot 2\text{H}_2\text{O}$                              | 219.07 | 2.75                                                | anhyd 200                   | d 698     | 9.2 g/100 mL <sup>25</sup> aq                                          |
| selenide               | CaSe                                                                    | 119.04 | 3.82                                                |                             |           |                                                                        |
| silicate               | $\text{Ca}_2\text{SiO}_4$                                               | 172.24 | 3.27                                                | 2130                        |           | i aq                                                                   |
| stearate               | $\text{Ca}(\text{C}_{18}\text{H}_{35}\text{O}_2)_2$                     | 607.04 |                                                     | 179–180                     |           | 0.004 <sup>15</sup> aq; s hot pyr; i acet, chl                         |
| succinate 3-water      | $\text{CaC}_4\text{H}_6\text{O}_4 \cdot 3\text{H}_2\text{O}$            | 212.22 |                                                     |                             |           | 1.28 <sup>20</sup> aq; s acids; i alc                                  |
| sulfate                | $\text{CaSO}_4$                                                         | 136.14 | 2.960                                               | 1460                        |           | 0.20 aq; s acids                                                       |
| sulfate hemihydrate    | $\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$                             | 145.15 |                                                     | anhyd 163                   |           | 0.3 <sup>20</sup> aq; s acids, glyc                                    |
| sulfate 2-water        | $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$                               | 172.17 | 2.32                                                | – 1.5 H <sub>2</sub> O, 128 | anhyd 163 | 0.26 <sup>20</sup> aq; s acid, glyc                                    |
| sulfide                | CaS                                                                     | 72.14  | 2.59                                                | 2525                        |           | 0.02 (d) aq; d acids                                                   |
| sulfite 2-water        | $\text{CaSO}_3 \cdot 2\text{H}_2\text{O}$                               | 156.17 |                                                     | anhyd 100                   |           | 0.004 aq; s acids d; sl s alc                                          |
| (±)tartarate 4-water   | $\text{CaC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$            | 260.21 |                                                     | anhyd 200                   |           | 0.0045 <sup>25</sup> aq; s acids; sl s alc                             |
| telluride              | CaTe                                                                    | 167.68 | 4.873                                               |                             |           |                                                                        |
| tetraborate            | $\text{CaB}_4\text{O}_7$                                                | 195.36 |                                                     |                             |           | s dil acids                                                            |
| tetrahydridoaluminate  | $\text{Ca}[\text{AlH}_4]_2$                                             | 102.10 |                                                     | ign moist air               |           | d viol aq, alc; i bz, eth                                              |
| thiocyanate 3-water    | $\text{Ca}(\text{SCN})_2 \cdot 3\text{H}_2\text{O}$                     | 210.29 |                                                     | d > 160                     |           | 150 g/100 mL aq; v s alc                                               |
| thioglycollate 3-water | $\text{Ca}(-\text{OOCCH}_2\text{S}-) \cdot 3\text{H}_2\text{O}$         | 184.24 |                                                     | – H <sub>2</sub> O, > 95    | d > 220   | s aq; v sl s alc, chl; i bz, eth                                       |
| thiosulfate 6-water    | $\text{CaS}_2\text{O}_3 \cdot 6\text{H}_2\text{O}$                      | 260.30 | 1.872                                               | d > 45                      |           | 92 g/100 mL <sup>25</sup> aq; i alc                                    |
| titanate               | $\text{CaTiO}_3$                                                        | 135.84 | 3.98                                                | 1980                        |           |                                                                        |
| tungstate(VI)(2–)      | $\text{CaWO}_4$                                                         | 287.93 | 6.062 <sup>20</sup>                                 |                             |           | 0.0032 aq; d hot acids                                                 |
| Californium-252        | Cf                                                                      | 252.1  |                                                     | 900                         |           |                                                                        |
| chloride               | $\text{CfCl}_3$                                                         | 358.5  | 5.88                                                |                             |           |                                                                        |
| Carbon (diamond)       | C                                                                       | 12.011 | 3.513                                               | 3500 <sup>63.5atm</sup>     | 3930      | i aq, alc                                                              |
| (graphite)             | C                                                                       |        | 2.267                                               | subl 3915–4020              |           |                                                                        |
| dioxide                | $\text{CO}_2$                                                           | 44.01  | c: 1.56 <sup>–79</sup><br>g: 1.975 g/L <sup>0</sup> | – 78.44 subl                |           | 88 mL/100 mL <sup>20</sup> aq                                          |
| diselenide             | $\text{CSe}_2$                                                          | 169.93 | 2.6626 <sup>25</sup> <sub>4</sub>                   | – 45.5                      | 125.1     | i aq; s acet, eth; misc CCl <sub>4</sub> ; d alc                       |
| disulfide              | $\text{CS}_2$                                                           | 76.14  | 1.2555                                              | – 111.6                     | 46.56     | FP – 30; 0.29 <sup>20</sup> aq; s alc, eth                             |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                        | Formula                                             | Formula weight | Density                                                | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                |
|-----------------------------|-----------------------------------------------------|----------------|--------------------------------------------------------|----------------------|----------------------|-------------------------------------------------------------------|
| Carbon ( <i>continued</i> ) |                                                     |                |                                                        |                      |                      |                                                                   |
| hydride (methane)           | CH <sub>4</sub>                                     | 16.04          | 0.415 <sup>-164</sup>                                  | -182.48              | -161.49              | s bz                                                              |
| monoxide                    | CO                                                  | 28.01          | lq: 0.814 <sup>-195</sup><br>g: 1.250 g/L <sup>0</sup> | -205.05              | -191.49              | 2.3 mL/100 mL <sup>20</sup> aq; 16 mL/100 ml<br>alc; s HOAc, EtAc |
| suboxide                    | C <sub>3</sub> O <sub>2</sub>                       | 68.03          | 1.114 <sub>4</sub> <sup>0</sup><br>2.985 g/L           | -111.3               | 6.8                  | d aq to malonic acid; sl s CS <sub>2</sub>                        |
| tetrabromide                | CBr <sub>4</sub>                                    | 331.65         | 3.42                                                   | 90.1                 | 190                  | i aq; s alc, chl, eth                                             |
| tetrachloride               | CCl <sub>4</sub>                                    | 153.82         | 1.589 <sub>25</sub> <sup>25</sup>                      | -22.9                | 76.7                 | 0.05 mL/100 mL aq; s alc, chl, eth                                |
| tetrafluoride               | CF <sub>4</sub>                                     | 88.00          | 1.96 <sup>-184</sup>                                   | -183.6               | -127.8               | sl s aq                                                           |
| tetraiodide                 | CI <sub>4</sub>                                     | 519.63         | 4.34 <sub>4</sub> <sup>20</sup>                        | 171                  | subl 130             | slowly hyd aq; s bz, chl, eth                                     |
| Carbonyl bromide            | COBr <sub>2</sub>                                   | 187.82         | 2.5                                                    |                      | 64.5                 | hyd aq                                                            |
| chloride                    | COCl <sub>2</sub>                                   | 98.92          | 4.340 g/L                                              | -127.9               | 8.2                  | hyd aq; s bz, HOAc                                                |
| fluoride                    | COF <sub>2</sub>                                    | 66.01          | lq: 1.139<br>g: 2.896 g/L                              | -114.0               | -83.1                | hyd aq                                                            |
| sulfide                     | COS                                                 | 60.07          | 2.636 g/L                                              | -138.81              | -50.23               | 54 mL/100 mL <sup>20</sup> aq; s alc, CS <sub>2</sub>             |
| Cerium                      | Ce                                                  | 140.11         | 6.773                                                  | 795                  | 3440                 | i aq; s acids                                                     |
| (III) bromide               | CeBr <sub>3</sub>                                   | 379.83         | 5.18                                                   | 733                  | 1460                 | s aq, alc                                                         |
| (III) chloride              | CeCl <sub>3</sub>                                   | 246.47         | 3.97 <sup>25</sup>                                     | 817                  | 1730                 | s aq, alc                                                         |
| (III) fluoride              | CeF <sub>3</sub>                                    | 197.11         | 6.157                                                  | 1430                 | 2327                 | i but slowly hyd aq; s H <sub>2</sub> SO <sub>4</sub>             |
| (IV) fluoride               | CeF <sub>4</sub>                                    | 216.11         | 4.77                                                   | d > 550              |                      | i aq                                                              |
| (III) iodide                | CeI <sub>3</sub>                                    | 520.83         |                                                        | 766                  | 1400                 | s aq                                                              |
| (III) nitrate 3-water       | Ce(NO <sub>3</sub> ) <sub>3</sub> 3H <sub>2</sub> O | 380.17         |                                                        | anhyd 150            | d 200                | 234 g/100 mL <sup>20</sup> aq                                     |
| (IV) oxide                  | CeO <sub>2</sub>                                    | 172.11         | 7.65                                                   | 2400                 |                      | i aq; s acids                                                     |
| (III) sulfate               | Ce <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>     | 568.42         | 3.912                                                  | d 1000               |                      | 9.72 g/100 mL <sup>21</sup> aq                                    |
| (IV) sulfate                | Ce(SO <sub>4</sub> ) <sub>2</sub>                   | 332.24         | 3.91                                                   | d 195                |                      | hyd aq; s dil H <sub>2</sub> SO <sub>4</sub>                      |
| Cesium                      | Cs                                                  | 132.9054       | 1.8785 <sup>15</sup>                                   | 28.44                | 668.2                | d aq; s acids                                                     |
| bromide                     | CsBr                                                | 212.81         | 4.44                                                   | 636                  | ≈1300                | 107 g/100 mL <sup>18</sup> aq; s alc; i acet                      |
| carbonate                   | Cs <sub>2</sub> CO <sub>3</sub>                     | 325.82         | 4.24                                                   | 792                  |                      | v s aq; 11 g/100 mL <sup>20</sup> alc; s eth                      |
| chloride                    | CsCl                                                | 168.36         | 3.99                                                   | 646                  | 1300                 | g/100 mL: 187 <sup>20</sup> aq; 34 <sup>25</sup> MeOH; v s<br>alc |
| fluoride                    | CsF                                                 | 151.90         | 4.115                                                  | 703                  | 1231                 | 322 g/100 mL <sup>18</sup> aq                                     |
| hydroxide                   | CsOH                                                | 149.91         | 3.68                                                   | 272                  | 990                  | 386 g/100 mL <sup>15</sup> aq; s alc                              |

|                       |                                                                |        |                                                        |         |                       |                                                                                   |
|-----------------------|----------------------------------------------------------------|--------|--------------------------------------------------------|---------|-----------------------|-----------------------------------------------------------------------------------|
| iodate                | CsIO <sub>3</sub>                                              | 307.81 | 4.934 <sup>20</sup>                                    | 565     |                       | 2.6 <sup>25</sup> aq                                                              |
| iodide                | CsI                                                            | 259.81 | 4.510                                                  | 621     | ≈1280                 | 76.5 g/100 mL <sup>20</sup> aq; s EtOH; i acet                                    |
| nitrate               | CsNO <sub>3</sub>                                              | 194.91 | 3.66                                                   | 414     | d 849                 | 23 g/100 mL <sup>20</sup> aq; s acet; v sl s alc                                  |
| oxide                 | Cs <sub>2</sub> O                                              | 281.81 | 4.65                                                   | 490     |                       | v s aq                                                                            |
| perchlorate           | CsClO <sub>4</sub>                                             | 232.36 | 3.327                                                  | 250     |                       | g/100 mL <sup>25</sup> : 1.96, 0.0086 EtOH, 0.118 acet, 0.0048 BuOH; i EtOAc, eth |
| selenate              | Cs <sub>2</sub> SeO <sub>4</sub>                               | 408.77 | 4.453                                                  |         |                       | 244 g/100 mL <sup>12</sup> aq                                                     |
| sulfate               | Cs <sub>2</sub> SO <sub>4</sub>                                | 361.87 | 4.243                                                  | 1005    |                       | 179 g/100 mL <sup>20</sup> aq; i alc, acet, pyr                                   |
| Chlorine              | Cl <sub>2</sub>                                                | 70.905 | g: 2.98 <sup>20</sup> g/L<br>lq: 1.5649 <sup>-35</sup> | -101.5  | -34.04                | 199 mL/100 mL <sup>25</sup> aq                                                    |
| dioxide               | ClO <sub>2</sub>                                               | 67.45  | 2.960 g/L                                              | -59.6   | 10.9                  | 11.2 g/100 mL <sup>10</sup> aq                                                    |
| fluoride              | ClF                                                            | 54.45  | 4.057 g/L                                              | -155.6  | -100.1                | d viol aq; organics burst into flame                                              |
| heptoxide             | Cl <sub>2</sub> O <sub>7</sub>                                 | 182.90 | 1.805 <sup>25</sup>                                    | -91.5   | 82                    | hyd aq slowly; explodes on concussion or on contact with flame or I <sub>2</sub>  |
| monoxide              | Cl <sub>2</sub> O                                              | 86.90  | 3.813 g/L                                              | -120.6  | 2.2                   | v s aq (forms HClO); s CCl <sub>4</sub>                                           |
| pentafluoride         | ClF <sub>5</sub>                                               | 130.44 | 5.724 g/L                                              | -103    | -13.1                 |                                                                                   |
| trifluoride           | ClF <sub>3</sub>                                               | 92.45  | g: 4.057 g/L<br>lq: 1.825 <sup>20</sup> g/L            | -76.3   | 11.75                 | hyd viol aq; organic matter and glass wool burst into flame                       |
| trioxide (dimer)      | (ClO <sub>3</sub> ) <sub>2</sub>                               | 166.90 | 1.92 <sup>20</sup>                                     | 3.5     | ≈200                  | reacts with aq                                                                    |
| Chromium              | Cr                                                             | 51.996 | 7.15                                                   | 1907    | 2679                  | s dil HCl                                                                         |
| (II) acetate          | Cr(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> | 170.09 | 1.79                                                   |         |                       | sl s aq, alc; s a; i eth                                                          |
| (III) acetate         | Cr(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>3</sub> | 229.13 |                                                        |         |                       | s aq                                                                              |
| (II) bromide          | CrBr <sub>2</sub>                                              | 211.80 | 4.236                                                  | 842     |                       | s aq, alc                                                                         |
| (III) bromide         | CrBr <sub>3</sub>                                              | 291.71 | 4.68                                                   |         |                       | s hot aq; v s alc                                                                 |
| (II) chloride         | CrCl <sub>2</sub>                                              | 122.90 | 2.88 <sup>25</sup>                                     | 814     | subl 1300             | v s aq                                                                            |
| (III) chloride        | CrCl <sub>3</sub>                                              | 158.35 | 2.87                                                   | 1152    | d > 1300              | s aq, alc (slow); i acet                                                          |
| (II) fluoride         | CrF <sub>2</sub>                                               | 89.99  | 3.79                                                   | 894     |                       | sl s aq; s hot HCl                                                                |
| (III) fluoride        | CrF <sub>3</sub>                                               | 108.99 | 3.8                                                    | 1400    |                       | aq, alc; s HF, HCl                                                                |
| (III) formate 6-water | Cr(CHO <sub>2</sub> ) <sub>3</sub> · 6H <sub>2</sub> O         | 295.15 |                                                        | d > 300 |                       | s aq                                                                              |
| hexacarbonyl          | Cr(CO) <sub>6</sub>                                            | 220.06 | 1.77                                                   | d 130   | explodes 210          | i aq, alc; s eth, chl                                                             |
| (III) hydroxide       | Cr(OH) <sub>3</sub>                                            | 101.02 |                                                        | d       |                       | i aq; s acids                                                                     |
| (III) nitrate 9-water | Cr(NO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O          | 400.15 | 1.80                                                   | 66      | d > 100               | 208 g/100 mL <sup>15</sup> aq; s alc                                              |
| (III) oxide           | Cr <sub>2</sub> O <sub>3</sub>                                 | 151.99 | 5.21                                                   | 2330    | ≈3000                 | i aq, alc; sl s acids, alkalis                                                    |
| (IV) oxide            | CrO <sub>2</sub>                                               | 84.00  | 4.89                                                   | 197     | -O <sub>2</sub> , 250 | i aq; s HNO <sub>3</sub>                                                          |
| (VI) oxide            | CrO <sub>3</sub>                                               | 99.99  | 2.70 <sup>25</sup>                                     | 198     | d 250                 | 61.7 g/100 mL aq; may ign organics                                                |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                          | Formula                                                                            | Formula weight | Density              | Melting point,<br>°C     | Boiling point,<br>°C | Solubility in<br>100 parts solvent                        |
|-------------------------------|------------------------------------------------------------------------------------|----------------|----------------------|--------------------------|----------------------|-----------------------------------------------------------|
| Chromium ( <i>continued</i> ) |                                                                                    |                |                      |                          |                      |                                                           |
| (III) phosphate               | CrPO <sub>4</sub>                                                                  | 146.97         | 4.6                  | >1800                    |                      | i aq, acids, aq reg                                       |
| potassium bissulfate          | CrK(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O                            | 499.41         | 1.826 <sup>25</sup>  | 89                       | anhyd 400            | 22 g/100 mL <sup>25</sup> aq; i alc                       |
| 12-water                      |                                                                                    |                |                      |                          |                      |                                                           |
| (II) sulfate 7-water          | CrSO <sub>4</sub> · 7H <sub>2</sub> O                                              | 274.17         |                      |                          |                      | 22.9 g/100 mL <sup>0</sup> aq; sl s alc                   |
| (III) sulfate 18-water        | Cr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 18H <sub>2</sub> O               | 716.45         | 1.7                  | d 100                    |                      | 220 g/100 mL <sup>20</sup> aq                             |
| Chromyl chloride              | CrO <sub>2</sub> Cl <sub>2</sub>                                                   | 154.90         | 1.9145 <sup>25</sup> | − 96.5                   | 117                  | d aq; s bz, chl, eth, CCl <sub>4</sub>                    |
| fluoride                      | CrO <sub>2</sub> F <sub>2</sub>                                                    | 121.99         |                      | 31.6 <sup>885mm</sup>    | subl 29.6            |                                                           |
| Cobalt                        | Co                                                                                 | 58.9332        | 8.90                 | 1494                     | 2927                 | i aq; s dil HNO <sub>3</sub>                              |
| (II) acetate 4-water          | Co(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 4H <sub>2</sub> O | 249.08         | 1.705 <sup>19</sup>  | anhyd 140                |                      | s aq; 2.1 g/100 mL <sup>15</sup> MeOH                     |
| (III) acetate                 | Co(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>3</sub>                     | 236.07         |                      | d > 100                  |                      | s aq, HOAc, alc                                           |
| (II) bromide                  | CoBr <sub>2</sub>                                                                  | 218.74         | 4.909 <sup>25</sup>  | 678 (in N <sub>2</sub> ) |                      | 112 g/100 mL <sup>20</sup> aq; s alc, acet                |
| (II) carbonate                | CoCO <sub>3</sub>                                                                  | 118.94         | 4.13                 | d                        |                      | 0.18 <sup>15</sup> aq; s hot acids                        |
| (II) chloride                 | CoCl <sub>2</sub>                                                                  | 129.84         | 3.367 <sup>25</sup>  | 735                      | 1049                 | 53 g/100 mL <sup>20</sup> aq; s alc, acet, eth, glyc, pyr |
| (II) chloride 6-water         | CoCl <sub>2</sub> · 6H <sub>2</sub> O                                              | 237.93         | 1.924                | anhyd 110                |                      | 97 g/100 mL <sup>20</sup> aq                              |
| (II) chromate                 | CoCrO <sub>4</sub>                                                                 | 174.93         | ≈ 4.0                | d                        |                      | i aq; s acids                                             |
| (II) cyanide                  | Co(CN) <sub>2</sub>                                                                | 110.97         | 1.872 <sup>25</sup>  | d 300                    |                      | 0.0042 <sup>18</sup> aq; s KCN                            |
| (II) fluoride                 | CoF <sub>3</sub>                                                                   | 96.93          | 4.46                 | 1127                     | ≈ 1400               | 1.36 <sup>20</sup> aq; s warm mineral acids               |
| (III) fluoride                | CoF <sub>3</sub>                                                                   | 115.93         | 3.88                 | 926                      |                      | d aq                                                      |
| (II) formate 2-water          | Co(CHO <sub>2</sub> ) <sub>2</sub> · 2H <sub>2</sub> O                             | 185.00         | 2.129 <sup>22</sup>  | anhyd 140                | d 175                | 5.03 g/100 mL <sup>30</sup> aq; i alc                     |
| (II) hydroxide                | Co(OH) <sub>2</sub>                                                                | 92.95          | 3.37                 | 168 (vacuo)              |                      | 0.00018 aq; v s acids                                     |
| (III) hydroxide               | Co(OH) <sub>3</sub>                                                                | 109.96         | 4.46                 | − H <sub>2</sub> O, 100  | d                    | 0.00032 aq; s acids                                       |
| (II) iodide (alpha, black)    | CoI <sub>2</sub>                                                                   | 312.74         | 5.584 <sup>25</sup>  | 515 (vacuo)              | 570 (vacuo)          | 203 aq                                                    |
| (II) nitrate 6-water          | Co(NO <sub>3</sub> ) <sub>3</sub> · 6H <sub>2</sub> O                              | 291.03         | 1.88                 | 55                       | d > 74               | 155 g/100 mL <sup>30</sup> aq; v s alc                    |
| (II) oxalate                  | CoC <sub>2</sub> O <sub>4</sub>                                                    | 146.95         | 3.021                | d 250                    |                      | 0.002 <sup>18</sup> aq                                    |
| (II) oxide                    | CoO                                                                                | 74.93          | 6.44                 | − s1935                  |                      | i aq; s acids, alkalis                                    |
| (II,III) oxide                | Co <sub>3</sub> O <sub>4</sub>                                                     | 240.80         | 6.07                 | d > 900                  |                      | i aq; s acids, alkalis                                    |
| (II) phosphate 8-water        | Co <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> · 8H <sub>2</sub> O                | 510.87         | 2.769                | anhyd 200                |                      | v sl s aq; s mineral acids                                |
| (II) sulfate 7-water          | CoSO <sub>4</sub> · 7H <sub>2</sub> O                                              | 281.10         | 2.03                 | anhyd 420                | d 1140               | 65 g/100 mL <sup>20</sup> aq; sl s alc                    |
| (II) sulfide                  | CoS                                                                                | 91.00          | 5.45 <sup>18</sup>   | 1180                     |                      | i aq; s acids                                             |
| (II) thiocyanate 3-water      | Co(SCN) <sub>2</sub> · 3H <sub>2</sub> O                                           | 229.14         |                      | anhyd 105                |                      | 7.8 <sup>18</sup> aq; s alc, eth                          |

|                                            |                                                                                                      |         |                                 |                          |                         |                                                            |
|--------------------------------------------|------------------------------------------------------------------------------------------------------|---------|---------------------------------|--------------------------|-------------------------|------------------------------------------------------------|
| Copper                                     | Cu                                                                                                   | 63.546  | 8.96 <sup>20</sup>              | 1084.62                  | 2561.5                  | i; s HNO <sub>3</sub> , hot H <sub>2</sub> SO <sub>4</sub> |
| (II) acetate 1-water                       | Cu(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O                    | 199.65  | 1.882                           | 115                      | d 240                   | 8 g/100 mL aq; 0.48 MeOH; sl s eth                         |
| acetate <i>meta</i> -arsenate (1/3)        | Cu(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 3Cu(AsO <sub>2</sub> ) <sub>2</sub> | 1013.80 |                                 |                          |                         | unstable in acids, bases; s NH <sub>4</sub> OH             |
| (II) borate(1–)                            | Cu(BO <sub>2</sub> ) <sub>2</sub>                                                                    | 149.17  | 3.859                           |                          |                         | s a; i aq                                                  |
| (I) bromide                                | CuBr                                                                                                 | 143.45  | 4.98                            | 497                      | 1345                    | v sl s aq; s HCl, HBr, NH <sub>4</sub> OH                  |
| (II) bromide                               | CuBr <sub>2</sub>                                                                                    | 223.35  | 4.71                            | 498                      | 900                     | 126 g/100 mL aq; s alc, acet, pyr; i bz                    |
| (II) carbonate hydroxide (1/1) (malachite) | CuCO <sub>3</sub> · Cu(OH) <sub>2</sub>                                                              | 221.12  | 4.0                             | d 200                    |                         | i aq; s acids                                              |
| (II) chlorate 6-water                      | Cu(ClO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                                               | 338.54  |                                 | 65                       | d 100                   | 242 g/100 mL <sup>18</sup> aq; v s alc; s acet             |
| (I) chloride                               | CuCl                                                                                                 | 99.00   | 4.14                            | 430                      | ≈1400                   | 0.024 aq; s conc HCl, conc NH <sub>4</sub> OH              |
| (II) chloride                              | CuCl <sub>2</sub>                                                                                    | 134.45  | 3.386                           | 300 d                    |                         | 73 g/100 mL <sup>20</sup> aq; s alc, acet                  |
| (II) chloride 2-water                      | CuCl <sub>2</sub> · 2H <sub>2</sub> O                                                                | 170.48  | 2.51                            | anhyd 200                | d >300                  | 76.4 g/100 mL <sup>25</sup> aq; v s alc; s acet            |
| (I) chromium(III) oxide (1/1)              | Cr <sub>2</sub> O <sub>3</sub> · Cu <sub>2</sub> O                                                   | 295.07  | 5.24 <sup>20</sup>              | d >900                   |                         | i aq; s HNO <sub>3</sub>                                   |
| (II) citrate 2.5-water                     | Cu <sub>2</sub> C <sub>6</sub> H <sub>4</sub> O <sub>7</sub> · 2.5H <sub>2</sub> O                   | 360.22  |                                 | anhyd 100                |                         | 0.17 aq; s acids                                           |
| (I) cyanide                                | CuCN                                                                                                 | 89.56   | 2.92                            | 473 (in N <sub>2</sub> ) | d                       | i aq; s NH <sub>4</sub> OH, KCN; d hot dil HCl             |
| (II) fluoride                              | CuF <sub>2</sub>                                                                                     | 101.54  | 4.23                            | 836                      | 1676                    | 4.75 g/100 mL <sup>20</sup> aq; s acids                    |
| (II) formate                               | Cu(CHO <sub>2</sub> ) <sub>2</sub>                                                                   | 153.58  | 1.831                           |                          |                         | 12.5 aq                                                    |
| (II) hexafluorosilicate 4-water            | Cu[SiF <sub>6</sub> ] · 4H <sub>2</sub> O                                                            | 277.60  | 2.56                            | d                        |                         | 124 g/100 mL <sup>20</sup> aq                              |
| (II) hydroxide                             | Cu(OH) <sub>2</sub>                                                                                  | 97.56   | 3.368                           | d 160                    |                         | i aq; s acids                                              |
| (I) iodide                                 | CuI                                                                                                  | 190.45  | 5.67                            | 606                      | ≈1290                   | i aq; s KCN, NH <sub>4</sub> OH, KI                        |
| (II) nitrate 3-water                       | Cu(NO <sub>3</sub> ) <sub>2</sub> · 3H <sub>2</sub> O                                                | 241.60  | 2.32                            | 114.5                    | 170 d                   | 138 g/100 mL <sup>0</sup> aq; v s alc                      |
| (II) oleate                                | Cu(OOCC <sub>17</sub> H <sub>33</sub> ) <sub>2</sub>                                                 | 626.46  |                                 |                          |                         | i aq; sl s alc; s eth                                      |
| (II) oxalate hemihydrate                   | CuC <sub>2</sub> O <sub>4</sub> · 0.5H <sub>2</sub> O                                                | 160.57  |                                 | anhydr >200              | d 310                   | 0.002 aq; s NH <sub>4</sub> OH                             |
| (I) oxide                                  | Cu <sub>2</sub> O                                                                                    | 143.09  | 6.0 <sub>4</sub> <sup>25</sup>  | 1235                     | – O <sub>2</sub> , 1800 | i aq; s HCl                                                |
| (II) oxide                                 | CuO                                                                                                  | 79.54   | 6.315 <sub>4</sub> <sup>4</sup> | 1450                     |                         | i aq, alc; s acids, KCN                                    |
| (II) perchlorate                           | Cu(ClO <sub>4</sub> ) <sub>2</sub>                                                                   | 262.45  | 2.225 <sup>23</sup>             | d >130                   |                         | 146 g/100 mL <sup>30</sup> aq; s eth, EtAc; i bz           |
| (II) phosphate 3-water                     | Cu <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> · 3H <sub>2</sub> O                                  | 434.63  |                                 | d                        |                         | i aq; s acids                                              |
| (II) salicylate 4-water                    | Cu(C <sub>7</sub> H <sub>5</sub> O <sub>3</sub> ) <sub>2</sub> · 4H <sub>2</sub> O                   | 409.83  |                                 | d                        |                         | v s aq; s alc                                              |
| (II) selenate 5-water                      | CuSeO <sub>4</sub> · 5H <sub>2</sub> O                                                               | 296.58  | 2.559                           | anhyd 265                | d ca. 480               | 25 g/100 mL <sup>20</sup> aq; v sl s acet                  |
| (I) selenide                               | Cu <sub>2</sub> Se                                                                                   | 206.05  | 6.84 <sub>4</sub> <sup>21</sup> | 1113                     |                         | d HCl                                                      |
| (II) selenide                              | CuSe                                                                                                 | 142.51  | 6.0                             | d 550                    |                         | s acids                                                    |
| (II) stearate                              | Cu(OOCC <sub>17</sub> H <sub>35</sub> ) <sub>2</sub>                                                 | 630.50  |                                 | ≈250                     |                         | i aq, alc, eth; s hot bz, pyr                              |
| (II) sulfate                               | CuSO <sub>4</sub>                                                                                    | 159.61  | 3.603                           | d >560                   |                         | 14.3 g/100 mL <sup>0</sup> aq; i alc                       |
| (II) sulfate 5-water                       | CuSO <sub>4</sub> · 5H <sub>2</sub> O                                                                | 249.69  | 2.284 <sub>4</sub> <sup>6</sup> | anhyd 200                |                         | 32 g/100 mL <sup>20</sup> aq; s MeOH, glyc                 |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                      | Formula                                                             | Formula weight | Density                        | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                                |
|---------------------------|---------------------------------------------------------------------|----------------|--------------------------------|----------------------|----------------------|-----------------------------------------------------------------------------------|
| <i>Copper (continued)</i> |                                                                     |                |                                |                      |                      |                                                                                   |
| (I) sulfide               | Cu <sub>2</sub> S                                                   | 159.16         | 5.6 <sub>4</sub> <sup>20</sup> | 1130                 |                      | i aq; d HNO <sub>3</sub> , s KCN                                                  |
| (II) sulfide              | CuS                                                                 | 95.61          | 4.76                           |                      |                      | i aq; s hot HNO <sub>3</sub> , KCN                                                |
| (I) sulfite hydrate       | Cu <sub>2</sub> SO <sub>3</sub> · H <sub>2</sub> O                  | 225.16         | 3.83 <sup>15</sup>             | d                    |                      | sl s aq; s HCl                                                                    |
| (II) tartrate 3-water     | CuC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 3H <sub>2</sub> O  | 265.66         |                                |                      |                      | 0.4220 aq; s acids, alkalis                                                       |
| (I) thiocyanate           | CuSCN                                                               | 121.62         | 2.85                           | 1084                 |                      | 0.00044 aq; s NH <sub>4</sub> OH, eth, alkali<br>SCN                              |
| (II) tungstate(VI)(2-)    | CuWO <sub>4</sub> · 2H <sub>2</sub> O                               | 347.41         |                                |                      |                      | 0.1 <sup>15</sup> aq; d acids; s NH <sub>4</sub> OH                               |
| Curium-244                | Cm                                                                  | 244.063        | 13.51                          | 1340                 | ≈3110                | s acids                                                                           |
| Cyanogen                  | NC—CN                                                               | 52.03          | 2.335 g/L                      | −27.84               | −21.15               | mL/100 mL: 450 <sup>20</sup> aq, 230 alc;                                         |
| azide                     | NC—N <sub>3</sub>                                                   | 68.04          |                                |                      |                      | s acetonitrile; pure azide detonates<br>upon shock. Handle only in sol-<br>vents. |
| bromide                   | NCBr                                                                | 105.92         | 2.005                          | 52                   | 61.5                 | v s aq, alc, eth                                                                  |
| chloride                  | NCCl                                                                | 61.47          | 2.697 g/L                      | −6.5                 | 13.8                 | s aq, alc, eth                                                                    |
| fluoride                  | NCF                                                                 | 45.02          | 1.975 g/L                      | −82                  | −46                  |                                                                                   |
| Deuterium                 | D <sub>2</sub> or <sup>2</sup> H <sub>2</sub>                       | 4.03           | 0.169 <sup>mp</sup> lq         | −252.89              | −249.49              | sl s aq                                                                           |
| oxide                     | D <sub>2</sub> O                                                    | 20.03          | 1.1056 <sup>20</sup>           | 3.82                 | 101.43               | misc aq                                                                           |
| Dysprosium                | Dy                                                                  | 162.50         | 8.540 <sup>25</sup>            | 1412                 | 2567                 | s acids                                                                           |
| bromide                   | DyBr <sub>3</sub>                                                   | 402.21         | 4.78                           | 880                  | 1480                 | s aq                                                                              |
| chloride                  | DyCl <sub>3</sub>                                                   | 268.86         | 3.67                           | 680                  | 1530                 | s aq                                                                              |
| fluoride                  | DyF <sub>3</sub>                                                    | 219.50         | 7.465                          | 1154                 | 2230                 | i aq                                                                              |
| oxide                     | Dy <sub>2</sub> O <sub>3</sub>                                      | 373.00         | 7.81 <sup>27</sup>             | 2408                 |                      | s aq                                                                              |
| Einsteinium               | Es                                                                  | 252.083        | 8.84                           | 860                  |                      |                                                                                   |
| Erbium                    | Er                                                                  | 167.26         | 9.066                          | 1529                 | 2868                 | s acid                                                                            |
| chloride                  | ErCl <sub>3</sub>                                                   | 273.62         | 4.1                            | 776                  | 1500                 | s aq; sl s alc                                                                    |
| oxide                     | Er <sub>2</sub> O <sub>3</sub>                                      | 382.52         | 8.640                          | 2418                 |                      | 0.0005 <sup>25</sup> aq; s acids                                                  |
| sulfate 8-water           | Er <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O | 766.83         | 3.205                          | anhyd 110            | d 630                | 16.0 g/100 mL <sup>20</sup> aq                                                    |
| Europium                  | Eu                                                                  | 151.965        | 5.244                          | 822                  | 1527                 | s acids                                                                           |
| (III) chloride            | EuCl <sub>3</sub>                                                   | 258.32         | 4.89                           | 623 d                |                      | s aq                                                                              |
| (III) oxide               | Eu <sub>2</sub> O <sub>3</sub>                                      | 351.93         | 7.42                           | 2350                 |                      | i aq; s acids                                                                     |
| (III) sulfate 8-water     | Eu <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O | 736.24         | −8H <sub>2</sub> O, 375        |                      |                      | 2.56 <sup>20</sup> aq                                                             |

|                       |                                                                     |          |                            |           |                                        |                                                                        |
|-----------------------|---------------------------------------------------------------------|----------|----------------------------|-----------|----------------------------------------|------------------------------------------------------------------------|
| Fermium-257           | Fm                                                                  | 257.0951 |                            | 1527      |                                        |                                                                        |
| Fluorine              | F <sub>2</sub>                                                      | 38.00    | 1.513 <sup>bp</sup> lq     | − 219.61  | − 188.13                               | d aq viol; ignites organics and silicates                              |
| nitrate               | FONO <sub>2</sub>                                                   | 81.00    | 1.667 g/L                  |           |                                        |                                                                        |
|                       |                                                                     |          | 1.507 <sup>bp</sup> lq     | − 175     | − 45.9                                 | hyd aq; s acet; ignites alc, eth; liquid explodes on slight concussion |
| perchlorate           | FOClO <sub>3</sub>                                                  | 118.45   | 5.20 g/L                   | − 167.3   | − 15.9                                 | explodes on slightest provocation                                      |
| Francium-223          | Fr                                                                  | 223.02   |                            |           |                                        |                                                                        |
| Gadolinium            | Gd                                                                  | 157.25   | 7.90                       | 1312      | 3273                                   | s acids                                                                |
| chloride              | GdCl <sub>3</sub>                                                   | 263.61   | 4.52 <sup>0</sup>          | ~ 609     | 1580                                   | s aq                                                                   |
| fluoride              | GdF <sub>3</sub>                                                    | 214.25   | 7.047                      | 1231      | 2277                                   | i aq                                                                   |
| nitrate 6-water       | Gd(NO <sub>3</sub> ) <sub>3</sub> · 6H <sub>2</sub> O               | 451.36   | 2.332                      | 91        |                                        | s aq, alc                                                              |
| oxide                 | Gd <sub>2</sub> O <sub>3</sub>                                      | 362.50   | 7.407 <sup>15</sup>        | 2340      |                                        | s acids                                                                |
| sulfate 8-water       | Gd <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> · 8H <sub>2</sub> O | 746.81   | 3.010 <sup>18</sup>        | anhyd 400 | d 500                                  | 4.08 aq                                                                |
| Gallium               | Ga                                                                  | 69.723   | 5.904 <sup>29.6</sup> (c)  | 29.7646   | 2203                                   | s conc HCl, halogens, alkalis                                          |
|                       |                                                                     |          | 6.095 <sup>29.8</sup> (lq) |           |                                        |                                                                        |
| antimonide            | GaSb                                                                | 191.48   | 5.614                      | 712       |                                        | s HCl                                                                  |
| arsenide              | GaAs                                                                | 144.65   | 5.318 <sup>25</sup>        | 1238      |                                        | s HCl                                                                  |
| chloride              | GaCl <sub>3</sub>                                                   | 176.08   | 2.47                       | 77.9      | 201.2                                  | d aq; s bz, CCl <sub>4</sub> , CS <sub>2</sub>                         |
| fluoride              | GaF <sub>3</sub>                                                    | 126.72   | 4.47                       | >1000     | subl 950                               | 0.004 <sup>25</sup> aq; s HF                                           |
| nitrate               | Ga(NO <sub>3</sub> ) <sub>3</sub>                                   | 255.74   |                            | d 110     | → Ga <sub>2</sub> O <sub>3</sub> , 200 | v s aq                                                                 |
| phosphide             | GaP                                                                 | 100.70   |                            | 1465      |                                        |                                                                        |
| selenide              | GaSe                                                                | 148.68   | 5.03 <sup>25</sup>         | 960       | d                                      |                                                                        |
| triethyl              | Ga(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>                     | 146.90   | 1.058 <sup>30</sup>        | − 82.3    | 142.8                                  |                                                                        |
| trimethyl             | Ga(CH <sub>3</sub> ) <sub>3</sub>                                   | 114.84   | 1.151 <sup>15</sup>        | − 15.7    | 55.8                                   |                                                                        |
| Germanium             | Ge                                                                  | 72.61    | 5.323                      | 937.3     | 2830                                   | i aq; s hot H <sub>2</sub> SO <sub>4</sub>                             |
| (IV) bromide          | GeBr <sub>4</sub>                                                   | 392.23   | 3.132                      | 26.1      | 186.4                                  | hyd aq; s bz, eth                                                      |
| (IV) chloride         | GeCl <sub>4</sub>                                                   | 214.42   | 1.879                      | − 49.5    | 86.5                                   | hyd aq; s bz, eth; sl s dil HCl                                        |
| (IV) fluoride         | GeF <sub>4</sub>                                                    | 148.60   | 6.521 g/L                  | − 15      | d > 1000                               | hyd aq; s dil HCl                                                      |
| hydride (germane)     | GeH <sub>4</sub>                                                    | 76.64    | 3.363 g/L                  | − 164.8   | − 88.1                                 | sl s hot HCl                                                           |
| (IV) oxide            | GeO <sub>2</sub>                                                    | 104.61   | 4.25                       | 1115      | 1200                                   | 0.43 <sup>20</sup> aq; s acids, alkalis                                |
| sulfide               | GeS <sub>2</sub>                                                    | 136.74   | 3.01                       | 530       |                                        |                                                                        |
| Gold                  | Au                                                                  | 196.967  | 19.3                       | 1064.18   | 2856                                   | s aq reg, KCN, hot H <sub>2</sub> SO <sub>4</sub>                      |
| (I) chloride          | AuCl                                                                | 232.42   | 7.57                       | 289       |                                        | s HCl, HBr, KCN                                                        |
| (III) chloride        | AuCl <sub>3</sub>                                                   | 303.33   | 4.7                        | d > 160   | subl 180                               | 68 g/100 mL <sup>20</sup> aq; s EtOH                                   |
| (I) cyanide           | AuCN                                                                | 222.99   | 7.14 <sup>20</sup>         | d         |                                        | s aq reg, KCN, NH <sub>4</sub> OH                                      |
| (III) cyanide 3-water | Au(CN) <sub>3</sub> · 3H <sub>2</sub> O                             | 329.07   |                            | d 50      |                                        | v s aq; sl s alc                                                       |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

3.30

| Name                              | Formula                                                                                       | Formula weight                          | Density                  | Melting point,<br>°C      | Boiling point,<br>°C | Solubility in<br>100 parts solvent      |
|-----------------------------------|-----------------------------------------------------------------------------------------------|-----------------------------------------|--------------------------|---------------------------|----------------------|-----------------------------------------|
| Gold ( <i>continued</i> )         |                                                                                               |                                         |                          |                           |                      |                                         |
| diantimonide                      | AuSb <sub>2</sub>                                                                             | 440.47                                  |                          | 460                       |                      |                                         |
| (III) fluoride                    | AuF <sub>3</sub>                                                                              | 253.96                                  | 6.75                     | subl 300                  | d 500                |                                         |
| (III) oxide                       | Au <sub>2</sub> O <sub>3</sub>                                                                | 441.93                                  |                          | d 150                     |                      | s HCl, KCN                              |
| (I) sodium thiosulfate<br>2-water | AuNa <sub>3</sub> (S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> · 2H <sub>2</sub> O           | 526.24                                  | 3.09                     | anhyd 160                 |                      | 50 g/100 mL aq; i alc                   |
| stannide                          | AuSn                                                                                          | 315.66                                  |                          | 418                       |                      |                                         |
| (III) sulfide                     | Au <sub>2</sub> S <sub>3</sub>                                                                | 490.13                                  | 8.754                    | d 197                     |                      | i aq; s Na <sub>2</sub> S               |
| Hafnium                           | Hf                                                                                            | 178.49                                  | 13.31                    | 2227                      | 4450                 | s HF                                    |
| chloride                          | HfCl <sub>4</sub>                                                                             | 320.30                                  |                          | 432                       | subl 317             | hyd aq; s acet, MeOH                    |
| oxide                             | HfO <sub>2</sub>                                                                              | 210.49                                  | 9.68 <sup>20</sup>       | 2774                      |                      | i aq                                    |
| Helium                            | He                                                                                            | 4.00260                                 | 0.176 g/L<br>0.1249 (lq) | − 272.15 <sup>25atm</sup> | − 268.935            | 0.861 mL/100 mL <sup>20</sup> aq        |
| Holmium                           | Ho                                                                                            | 164.9304                                | 8.79                     | 1474                      | 2720                 | s acids; oxidizes in moist air          |
| bromide                           | HoBr <sub>3</sub>                                                                             | 404.64                                  | 4.86                     | 914                       | 1470                 | s aq                                    |
| chloride                          | HoCl <sub>3</sub>                                                                             | 271.29                                  | 3.7                      | 718                       | 1510                 | s aq                                    |
| Hydrazine                         | H <sub>2</sub> N—NH <sub>2</sub>                                                              | 32.05                                   | 1.0036 <sup>25</sup>     | 2.0                       | 113.5                | FP 52; misc aq, alc                     |
| hydrate                           | H <sub>2</sub> N—NH <sub>2</sub> · H <sub>2</sub> O                                           | 50.06                                   | 1.030                    | − 51.7 & − 65             | 118–119              | misc aq, alc; i chl, eth                |
| Hydrazinium(1+) chloride          | H <sub>2</sub> N—NH <sub>3</sub> Cl                                                           | 68.51                                   | 1.5                      | 89                        | d 240                | v s aq; i org solv                      |
| (2+) chloride                     | ClH <sub>3</sub> N—NH <sub>3</sub> Cl                                                         | 104.97                                  | 1.423                    | 198                       | d 200                | v s aq; sl s alc                        |
| (1+) iodide                       | H <sub>2</sub> N—NH <sub>3</sub> I                                                            | 159.96                                  |                          | 125                       |                      | s aq                                    |
| (+1) perchlorate                  | H <sub>2</sub> N—NH <sub>3</sub> ClO <sub>4</sub>                                             | 132.51                                  | 1.939 <sup>15</sup>      | 137                       | d 145                | d aq; s alc                             |
| (2+) sulfate                      | (H <sub>3</sub> NNH <sub>3</sub> )SO <sub>4</sub>                                             | 130.13                                  | 1.378                    | 254                       | d                    | 3.4 <sup>20</sup> aq; i alc             |
| (1+) tartrate                     | (H <sub>2</sub> N—NH <sub>3</sub> ) <sub>2</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> | 182.13                                  |                          | 183                       |                      | 6.0 g/100 mL <sup>0</sup> aq            |
| Hydrogen                          | H <sub>2</sub>                                                                                | 2.0159<br>0.07099 <sup>bp</sup><br>(lq) | 0.088 g/L                | − 259.35                  | − 252.88             | 1.9 mL aq                               |
| amidosulfate (sulfamate)          | H <sub>2</sub> NSO <sub>3</sub> H                                                             | 97.09                                   | 2.126                    | 205                       | d                    | 14.7 g/100 mL aq; sl s alc, acet        |
| azide                             | HN <sub>3</sub>                                                                               | 43.03                                   | 1.126 <sup>0</sup>       | − 80                      | 37                   | v s aq; (very explosive)                |
| borate(1−) (cubic)                | HBO <sub>2</sub>                                                                              | 43.83                                   | 2.486                    | 236                       |                      | v sl s aq                               |
| borate(3−) (ortho)                | H <sub>3</sub> BO <sub>3</sub>                                                                | 61.83                                   | 1.435 <sup>15</sup>      | 171.0                     | d 357                | 5.56 g/100 mL <sup>30</sup> aq          |
| bromide                           | HBr                                                                                           | 80.91                                   | 3.388 g/L <sup>20</sup>  | − 86.87                   | − 66.71              | 193 g/100 mL <sup>25</sup> aq; misc alc |



|                              |                                                        |        |                                   |                                      |                                                    |                                                      |
|------------------------------|--------------------------------------------------------|--------|-----------------------------------|--------------------------------------|----------------------------------------------------|------------------------------------------------------|
| bromide (constant boiling)   | 48% HBr + H <sub>2</sub> O                             |        | 1.49                              | − 11                                 | 126                                                | v s aq                                               |
| bromide- <i>d</i>            | <sup>2</sup> HBr                                       | 81.91  | 3.39 g/L <sup>20</sup>            | − 87.46                              | − 66.5                                             | v s aq                                               |
| bromosulfate                 | HOSO <sub>2</sub> Br                                   | 240.90 |                                   | − 6 to − 8                           | d                                                  | hyd aq                                               |
| chlorate (40% solution)      | HClO <sub>3</sub>                                      | 84.46  | 1.282 <sub>4</sub> <sup>0</sup>   |                                      |                                                    |                                                      |
| chloride                     | HCl                                                    | 36.46  | 1.526 g/L <sup>20</sup>           | − 114.18                             | − 85.05                                            | 72 g/100 mL <sup>20</sup> aq                         |
| chloride (constant boiling)  | 20.24% HCl + H <sub>2</sub> O                          |        | 1.097                             |                                      | 110                                                | v s aq                                               |
| chloride- <i>d</i>           | <sup>2</sup> HCl                                       | 37.47  | 1.49 g/L <sup>25</sup>            | − 114.64                             | − 84.72                                            | v s aq                                               |
| chlorosulfate                | HSO <sub>3</sub> Cl                                    | 116.52 | 1.753                             | − 80                                 | 152                                                | hyd viol → HCl + H <sub>2</sub> SO <sub>4</sub>      |
| cyanate                      | HOCN                                                   | 43.03  | 1.140 <sub>4</sub> <sup>−20</sup> | − 86                                 | 23.5                                               | s aq d; s bz, eth                                    |
| cyanide                      | HCN                                                    | 27.03  | 0.687                             | − 13.4                               | 25.6                                               | misc aq                                              |
| deuteride                    | <sup>1</sup> H <sup>2</sup> H or HD                    | 3.02   |                                   | − 256.56                             | − 251.03                                           |                                                      |
| diphosphate(IV)              | (HO) <sub>2</sub> OP—PO(OH) <sub>2</sub>               | 162.01 | 70                                | d 100                                | d                                                  | aq                                                   |
| diphosphate(V)               | H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>           | 177.98 |                                   | 61                                   |                                                    | 709 g/100 mL <sup>23</sup> aq                        |
| fluoride                     | HF                                                     | 20.01  | 0.922 g/L <sup>0</sup>            | − 83.57                              | 19.52                                              | v s aq, alc; 2.54 g/100 g <sup>5</sup> bz            |
| fluoride (constant boiling)  | 35.35% HF + H <sub>2</sub> O                           |        |                                   |                                      | 120                                                | v s aq                                               |
| fluoride- <i>d</i>           | <sup>2</sup> HF                                        | 21.02  |                                   | − 83.6                               | 18.65                                              | s aq                                                 |
| fluoroborate                 | H[BF <sub>4</sub> ]                                    | 87.81  |                                   | d 130                                |                                                    | v s aq                                               |
| fluorophosphate              | H <sub>2</sub> PO <sub>3</sub> F                       | 99.99  | 1.818                             | − 80                                 |                                                    |                                                      |
| fluorosulfate                | HOSO <sub>2</sub> F                                    | 100.07 | 1.726 <sub>4</sub> <sup>25</sup>  | − 87.3                               | 165.5                                              | s aq                                                 |
| hexafluorosilicate 2-water   | H <sub>2</sub> [SiF <sub>6</sub> ] · 2H <sub>2</sub> O | 180.11 | 1.463                             | 19                                   |                                                    | 60–70% aq solution                                   |
| iodate                       | HIO <sub>3</sub>                                       | 175.91 | 4.629 <sub>0</sub> <sup>4</sup>   | 110 → H <sub>5</sub> IO <sub>6</sub> | 220 → I <sub>2</sub> O <sub>5</sub>                | 269 g/100 mL <sup>20</sup> aq; s alc; i eth          |
| iodide                       | HI                                                     | 127.91 | 5.37 g/L <sup>20</sup>            | − 50.8                               | − 35.1                                             | 234 g/100 mL <sup>10</sup> aq; misc alc              |
| iodide (constant boiling)    | 57% HI + H <sub>2</sub> O                              |        | 1.70                              |                                      | 127                                                | v s aq                                               |
| iodide- <i>d</i>             | HI                                                     | 128.91 |                                   | − 51.87                              | − 35.7                                             | v s aq                                               |
| molybdate hydrate            | H <sub>2</sub> MoO <sub>4</sub> · H <sub>2</sub> O     | 179.97 | 3.124 <sup>15</sup>               | − H O, 70                            |                                                    | 0.133 <sup>18</sup> aq; s alk                        |
| nitrate                      | HNO <sub>3</sub>                                       | 63.02  | 1.5492 <sup>0</sup> lq            | − 41.59                              | 83                                                 | v s                                                  |
| nitrate (constant boiling)   | 69% HNO <sub>3</sub> + H <sub>2</sub> O                |        | 1.41 <sup>20</sup>                |                                      | 120.5                                              | misc aq                                              |
| oxide (water)                | H <sub>2</sub> O                                       | 18.02  | 1.000                             | 0.00                                 | 100.00                                             |                                                      |
| oxide- <i>d</i> <sub>2</sub> | D <sub>2</sub> O or <sup>2</sup> H <sub>2</sub> O      | 20.03  | 1.1044 <sup>25</sup>              | 3.81                                 | 101.42                                             | misc aq                                              |
| perchlorate 2-water          | HClO <sub>4</sub> · 2H <sub>2</sub> O                  | 136.49 | 1.67 <sup>20</sup>                | − 17.8                               | 203                                                | v s aq (commercial 72% acid)                         |
| periodate(1−) (meta)         | HIO <sub>4</sub>                                       | 191.91 |                                   | subl 110                             | d 138                                              | 440 g/100 mL <sup>25</sup> aq                        |
| periodate(5−)                | H <sub>5</sub> IO <sub>6</sub>                         | 227.94 |                                   | 122                                  | d 130–140                                          | misc aq; s alc                                       |
| peroxide                     | H <sub>2</sub> O <sub>2</sub>                          | 34.01  | 1.463 <sup>0</sup>                | − 0.43                               | 152                                                | misc aq; s alc, eth                                  |
| peroxodisulfate              | HO <sub>3</sub> S—O—OSO <sub>3</sub> H                 | 194.14 |                                   | d 60                                 |                                                    | v s aq                                               |
| phosphate(V)(1−) (meta)      | HPO <sub>3</sub>                                       | 79.98  | 2.2–2.5                           | subl                                 | red heat                                           | slowly s aq → H <sub>3</sub> PO <sub>4</sub> ; s alc |
| phosphate(V)(3−) (ortho)     | H <sub>3</sub> PO <sub>4</sub>                         | 98.00  | 1.868 <sup>25</sup>               | 42.35                                | d 213                                              | v s aq                                               |
| commercial 85% acid          |                                                        |        | 1.685                             | anhyd 150                            | H <sub>4</sub> P <sub>2</sub> O <sub>7</sub> , 200 | → HPO <sub>3</sub> , >300                            |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| 3.32 | Name                            | Formula                                                                       | Formula weight | Density                           | Melting point,<br>°C    | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                                                                         |
|------|---------------------------------|-------------------------------------------------------------------------------|----------------|-----------------------------------|-------------------------|----------------------|----------------------------------------------------------------------------------------------------------------------------|
|      |                                 |                                                                               |                |                                   |                         |                      |                                                                                                                            |
|      | Hydrogen ( <i>continued</i> )   |                                                                               |                |                                   |                         |                      |                                                                                                                            |
|      | phosphate(V)(3-)-d <sub>3</sub> | <sup>2</sup> H <sub>3</sub> PO <sub>4</sub>                                   | 101.03         | 1.908 <sup>25</sup>               | 46.0                    |                      | v s aq                                                                                                                     |
|      | phosphide, <i>see</i> Phosphine |                                                                               |                |                                   |                         |                      |                                                                                                                            |
|      | phosphinate                     | HPH <sub>2</sub> O <sub>2</sub>                                               | 66.0           | 1.493 <sup>19</sup>               | 26.5                    | d 50                 | s aq                                                                                                                       |
|      | phosphonate (phosphorous acid)  | H <sub>2</sub> PHO <sub>3</sub>                                               | 82.00          | 1.651 <sup>25</sup> <sub>4</sub>  | ≈ 73                    | d > 180              | v s aq, alc                                                                                                                |
|      | selenate                        | H <sub>2</sub> SeO <sub>4</sub>                                               | 144.98         | 2.9508 <sup>15</sup> <sub>4</sub> | 58                      | 260                  | vs aq (viol)                                                                                                               |
|      | selenide                        | H <sub>2</sub> Se                                                             | 80.98          | 2.12 <sub>4</sub> <sup>-bp</sup>  | -65.73                  | -41.4                | 9.5 mL/100 mL <sup>20</sup> aq; s CS <sub>2</sub>                                                                          |
|      | sulfate                         | H <sub>2</sub> SO <sub>4</sub>                                                | 98.08          | 1.8318 <sup>20</sup>              | 10.38                   | 335.5                | misc aq                                                                                                                    |
|      | sulfate-d <sub>2</sub>          | <sup>2</sup> H <sub>2</sub> SO <sub>4</sub> or D <sub>2</sub> SO <sub>4</sub> | 100.09         | 1.8620                            | 14.35                   |                      | misc aq                                                                                                                    |
|      | sulfide                         | H <sub>2</sub> S                                                              | 34.08          | 1.5392 g/L <sup>0</sup>           | -85.49                  | -60.33               | 0.334 mL <sup>25</sup> aq                                                                                                  |
|      | tellurate(IV)                   | H <sub>2</sub> TeO <sub>3</sub>                                               | 177.63         | 3.0                               | d to TeO <sub>2</sub>   |                      | 0.0007 aq; s acid, alkali                                                                                                  |
|      | tellurate(VI) (monoclinic)      | H <sub>6</sub> TeO <sub>6</sub>                                               | 229.66         | 3.068                             | -2H <sub>2</sub> O, 120 | 320 → TeO            | 30 g/100 mL <sup>18</sup> aq                                                                                               |
|      | telluride                       | H <sub>2</sub> Te                                                             | 129.62         | 5.687 g/L                         | -49                     | -2                   | s aq d                                                                                                                     |
|      | trithiocarbonate                | (HS) <sub>2</sub> CS                                                          | 110.21         | 1.483 <sup>20</sup> <sub>4</sub>  | -26.9                   | 57.8                 | d aq, alc                                                                                                                  |
|      | tungstate(VI)(2-)               | H <sub>2</sub> WO <sub>4</sub>                                                | 249.86         | 5.5                               | anhyd 100               |                      | i aq; s HF, alkalis                                                                                                        |
|      | Hydroxylamine                   | HONH <sub>2</sub>                                                             | 33.03          | 1.204 <sup>40</sup> <sub>4</sub>  | 33                      | 58 <sup>22mm</sup>   | v s aq, MeOH; sl s bz, eth                                                                                                 |
|      | Hydroxylammonium chloride       | HONH <sub>3</sub> Cl                                                          | 69.49          | 1.680 <sup>20</sup>               | 150.5                   | d                    | g/100 mL: 83 <sup>17</sup> aq, 12.5 <sup>20</sup> MeOH, 5.1 <sup>20</sup> EtOH; s glyc                                     |
|      | sulfate                         | (HONH <sub>3</sub> ) <sub>2</sub> SO <sub>4</sub>                             | 164.14         |                                   | 170                     |                      | 69 g/100 mL <sup>20</sup> aq                                                                                               |
|      | Indium                          | In                                                                            | 114.82         | 7.31                              | 156.60                  | 2072                 | s acids                                                                                                                    |
|      | antimonide                      | InSb                                                                          | 236.58         | 5.77                              | 525                     |                      | i aq                                                                                                                       |
|      | arsenide                        | InAs                                                                          | 189.74         | 5.67                              | 942                     |                      |                                                                                                                            |
|      | chloride                        | InCl <sub>3</sub>                                                             | 221.18         | 4.0                               | 583                     | subl 500             | 212 g/100 mL <sup>25</sup> aq                                                                                              |
|      | fluoride                        | InF <sub>3</sub>                                                              | 171.82         | 4.39                              | 1170                    |                      | 0.040 <sup>25</sup> aq; s dilute acids                                                                                     |
|      | oxide                           | In <sub>2</sub> O <sub>3</sub>                                                | 277.63         | 7.179                             |                         | 850                  | s hot mineral acids                                                                                                        |
|      | phosphide                       | InP                                                                           | 145.79         | 4.81                              | 1062                    |                      | v sl s acids                                                                                                               |
|      | telluride                       | In <sub>2</sub> Te <sub>3</sub>                                               | 612.44         | 5.75                              | 667                     |                      |                                                                                                                            |
|      | trimethyl                       | In(CH <sub>3</sub> ) <sub>3</sub>                                             | 159.93         | 1.568                             | 88.4                    | 135.8                | d aq; s acet, bz                                                                                                           |
|      | Iodine                          | I <sub>2</sub>                                                                | 253.809        | 4.63 <sup>25</sup>                | 113.60                  | 185.24               | g/100 mL <sup>25</sup> : 0.029 aq, 14.1 bz, 16.5 CS <sub>2</sub> , 21.4 EtOH, 25.2 eth, 2.6 CCl <sub>4</sub> ; s chl, HOAc |

|                            |                                                                     |         |                                  |                                    |           |                                                                 |
|----------------------------|---------------------------------------------------------------------|---------|----------------------------------|------------------------------------|-----------|-----------------------------------------------------------------|
| heptafluoride              | IF <sub>7</sub>                                                     | 259.89  | lq: 2.8 <sup>6</sup>             | 6.45                               | 4.77 subl | s aq (d), s NaOH                                                |
| monobromide                | IBr                                                                 | 206.81  | 4.416                            | 40                                 | 116 d     | s aq, alc, eth, CS <sub>2</sub>                                 |
| monochloride               | ICl                                                                 | 162.36  | 3.10 <sub>4</sub> <sup>29</sup>  | 27.2 α-form                        | 97 d      | d aq; s alc, eth, HOAc                                          |
| pentafluoride              | IF <sub>5</sub>                                                     | 221.90  | 3.19 <sup>25</sup>               | 9.43                               | 100.5     | d aq viol                                                       |
| pentoxide                  | I <sub>2</sub> O <sub>5</sub>                                       | 333.81  | 4.98                             | d 275                              |           | 187 g/100 mL <sup>13</sup> aq                                   |
| trichloride                | ICl <sub>3</sub>                                                    | 233.26  | 3.202 <sup>-4</sup>              | ~ 33                               | 64 subl   | d aq; s alc, bz, HCl                                            |
| Iridium                    | Ir                                                                  | 192.217 | 22.65 <sub>4</sub> <sup>20</sup> | 2447                               | ~ 2550    | s K <sub>2</sub> SO <sub>4</sub> fusion, KOH + KNO <sub>3</sub> |
|                            |                                                                     |         |                                  |                                    |           | fusion                                                          |
| hexafluoride               | IrF <sub>6</sub>                                                    | 306.21  | 4.82                             | 44.4                               | 53.6      | d aq                                                            |
| (III) oxide                | Ir <sub>2</sub> O <sub>3</sub>                                      | 432.43  |                                  | d ~ 1000 to Ir<br>+ O <sub>2</sub> |           | s boiling HCl                                                   |
| (IV) oxide                 | IrO <sub>2</sub>                                                    | 224.22  | 11.7                             | d 1100                             |           | 0.0002 <sup>20</sup> aq; s HCl                                  |
| trichloride                | IrCl <sub>3</sub>                                                   | 298.58  | 5.30                             | d 763                              |           | i acids, alkalis                                                |
| Iron                       | Fe                                                                  | 55.845  | 7.86                             | 1535                               | 2861      | i aq; s acids                                                   |
| (III) arsenate 2-water     | FeAsO <sub>4</sub> · 2H <sub>2</sub> O                              | 230.79  | 3.18                             | 1020                               |           | v sl s aq; s acids                                              |
| (II) bromide               | FeBr <sub>2</sub>                                                   | 126.75  | 3.16                             | 677                                | 1023      | 117 g/100 mL <sup>20</sup> aq; v s alc                          |
| (III) bromide              | FeBr <sub>3</sub>                                                   | 295.67  | 4.5                              | d                                  |           | s aq, alc, eth, HOAc                                            |
| (tri-) carbide             | Fe <sub>3</sub> C                                                   | 179.55  | 7.694                            | 1227                               |           | s acids                                                         |
| (II) carbonate             | FeCO <sub>3</sub>                                                   | 115.85  | 3.9                              | d                                  |           | 0.072 <sup>18</sup> aq; s acids                                 |
| (II) chloride              | FeCl <sub>2</sub>                                                   | 126.75  | 3.16                             | 677                                | 1024      | 62.5 g/100 mL <sup>20</sup> aq; v s alc, acet                   |
| (III) chloride             | FeCl <sub>3</sub>                                                   | 162.20  | 2.898                            | 304                                | ≈ 316     | 74 g/100 mL <sup>9</sup> aq; s alc, acet, eth                   |
| disulfide (pyrite)         | FeS <sub>2</sub>                                                    | 119.98  | 5.02                             | d 602                              |           | s acids d                                                       |
| (II) fluoride              | FeF <sub>2</sub>                                                    | 93.84   | 4.09                             | 1100                               | 1837      | sl s aq; s dil HF; i alc, bz, eth                               |
| (III) fluoride             | FeF <sub>3</sub>                                                    | 112.84  | 3.87                             | subl 1000                          |           | 0.091 <sup>25</sup> aq; s HF                                    |
| (III) hexacyanoferrate(II) | Fe <sub>4</sub> [Fe(CN) <sub>6</sub> ] <sub>3</sub>                 | 859.23  | 1.80                             | 250 d                              |           | i aq; s HCl                                                     |
| (II) hydroxide             | Fe(OH) <sub>2</sub>                                                 | 89.86   | 3.4                              |                                    |           | 0.006 aq; s acids                                               |
| (III) hydroxide oxide      | FeO(OH)                                                             | 88.85   | 4.26                             | anhyd 136                          |           | i aq, alc; s HCl                                                |
| (II) iodide                | FeI <sub>2</sub>                                                    | 309.65  | 5.315                            | 587                                | 1093      | s aq                                                            |
| (III) nitrate 9-water      | Fe(NO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O               | 404.00  | 1.684                            | 47                                 | d 100     | 138 g/100 mL <sup>20</sup> aq                                   |
| (di-) nitride              | Fe <sub>2</sub> N                                                   | 125.70  | 6.35                             | d 200                              |           | s HCl                                                           |
| (II) oxalate 2-water       | FeC <sub>2</sub> O <sub>4</sub> · 2H <sub>2</sub> O                 | 179.89  | 2.28                             | d 150                              |           | 0.044 <sup>18</sup> aq; s mineral acids                         |
| (II) oxide                 | FeO                                                                 | 71.84   | 6.0                              | 1377                               | d 3414    | i aq; s acids                                                   |
| (II,III) oxide             | Fe <sub>3</sub> O <sub>4</sub>                                      | 231.53  | 5.17                             | 1597                               |           | i aq; s acids                                                   |
| (III) oxide                | Fe <sub>2</sub> O <sub>3</sub>                                      | 159.69  | 5.25                             | 1565                               |           | i aq; s HCl                                                     |
| pentacarbonyl              | Fe(CO) <sub>5</sub>                                                 | 195.90  | 1.49                             | – 20.0                             | 103.9     | FP – 20; i aq; s alc, bz, eth                                   |
| (II) phosphate 8-water     | Fe <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> · 8H <sub>2</sub> O | 501.60  | 2.58                             |                                    |           | i aq; s acids                                                   |
| phosphide                  | Fe <sub>2</sub> P                                                   | 142.66  | 6.85                             | 1370                               |           | s hot mineral acids                                             |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

3.34

| Name                      | Formula                                                                            | Formula weight | Density                   | Melting point,<br>°C        | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                |
|---------------------------|------------------------------------------------------------------------------------|----------------|---------------------------|-----------------------------|----------------------|-------------------------------------------------------------------|
| Iron ( <i>continued</i> ) |                                                                                    |                |                           |                             |                      |                                                                   |
| (II) selenide             | FeSe                                                                               | 134.81         | 6.78                      | d                           |                      | s HCl                                                             |
| (II) silicate(2−)         | FeSiO <sub>3</sub>                                                                 | 131.93         | 3.5                       | 1140                        |                      |                                                                   |
| (II) silicate(4−)         | Fe <sub>2</sub> SiO <sub>4</sub>                                                   | 203.77         | 4.30                      | 1220                        |                      | d HCl                                                             |
| (II) sulfate 7-water      | FeSO <sub>4</sub> · 7H <sub>2</sub> O                                              | 278.01         | 1.89                      | anhyd 300                   | d 671                | 48 g/100 mL <sup>20</sup> aq                                      |
| (III) sulfate             | Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                                    | 399.88         | 3.097 <sup>18</sup>       | d 1178                      |                      | slowly s aq (hyd); sl s alc                                       |
| (II) sulfide              | FeS                                                                                | 87.92          | 4.7                       | 1190                        | d                    | 0.0006 <sup>18</sup> aq; s acid                                   |
| (III) thiocyanate         | Fe(SCN) <sub>3</sub>                                                               | 230.09         |                           |                             |                      | v s aq                                                            |
| Krypton                   | Kr                                                                                 | 83.80          | 3.7493 g/L                | − 157.36                    | − 153.22             | 5.94 mL/100 mL <sup>20</sup> aq                                   |
| difluoride                | KrF <sub>2</sub>                                                                   | 121.80         | 3.24                      | subl − 60                   |                      | s anhyd HF                                                        |
| Lanthanum                 | La                                                                                 | 138.9055       | 6.162                     | 920                         | 3464                 | i aq; s HCl                                                       |
| chloride                  | LaCl <sub>3</sub>                                                                  | 245.26         | 3.84                      | 852                         | 1812                 | v s aq                                                            |
| chloride 7-water          | LaCl <sub>3</sub> · 7H <sub>2</sub> O                                              | 371.37         |                           | anhyd 852 (in<br>HCl atm)   |                      | v s aq; s alc                                                     |
| fluoride                  | LaF <sub>3</sub>                                                                   | 195.90         | 5.9                       | 1493                        | 2327                 |                                                                   |
| nitrate 6-water           | La(NO <sub>3</sub> ) <sub>3</sub> · 6H <sub>2</sub> O                              | 433.01         |                           | 40                          | d 126                | 181 g/100 mL <sup>20</sup> aq; v s alc                            |
| oxide                     | La <sub>2</sub> O <sub>3</sub>                                                     | 325.81         | 6.51                      | 2305                        | 4200                 | s acids                                                           |
| sulfate                   | La <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                                    | 566.00         | 3.60                      | d white heat                |                      | 2.33 g/100 mL <sup>20</sup> aq; i alc                             |
| sulfate 9-water           | La <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 9H <sub>2</sub> O                | 728.14         | 2.821                     | anhyd 400                   |                      | 2.92 g/100 mL <sup>20</sup> aq; i alc                             |
| Lawrencium                | Lr                                                                                 | 262            |                           | 1627                        |                      |                                                                   |
| Lead                      | Pb                                                                                 | 207.2          | 11.34 <sup>20</sup> (fcc) | 327.43                      | 1749                 | s hot conc HNO <sub>3</sub> , HCl, H <sub>2</sub> SO <sub>4</sub> |
| (II) acetate 3-water      | Pb(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 3H <sub>2</sub> O | 427.3          | 2.55                      | 75                          | d > 200              | g/100 mL: 63 <sup>15</sup> aq, 3.3 alc                            |
| (IV) acetate              | Pb(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>4</sub>                     | 443.4          | 2.228                     | ≈ 75–180                    |                      | s hot HOAc, bz, chl, conc HX acids                                |
| (II) azide                | Pb(N <sub>3</sub> ) <sub>2</sub>                                                   | 291.2          | 4.7                       | expl 350 or<br>when shocked |                      | 0.023 <sup>18</sup> aq; v s HOAc                                  |
| (II) borate(1−) hydrate   | Pb(BO <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O                               | 310.8          | 5.598 anhyd               | anhyd 160                   | mp 500               | s acids                                                           |
| (II) bromide              | PbBr <sub>2</sub>                                                                  | 367.0          | 6.69                      | 371                         | 912                  | 0.450 <sup>0</sup> aq; s acids; i alc                             |
| (II) carbonate            | PbCO <sub>3</sub>                                                                  | 267.2          | 6.61                      | d 340 → PbO                 |                      | i aq; s acids, alkalis                                            |
| (II) chlorate             | Pb(ClO <sub>3</sub> ) <sub>2</sub>                                                 | 374.1          | 3.89                      | d 230                       |                      | 140 g/100 mL <sup>18</sup> aq; v s alc                            |
| (II) chloride             | PbCl <sub>2</sub>                                                                  | 278.1          | 5.98                      | 501                         | 950                  | 0.99 <sup>20</sup> aq                                             |
| (II) chloride fluoride    | PbClF                                                                              | 261.7          | 7.05                      |                             |                      |                                                                   |

|                          |                                                                    |        |                     |                                                            |             |                                                                                                             |
|--------------------------|--------------------------------------------------------------------|--------|---------------------|------------------------------------------------------------|-------------|-------------------------------------------------------------------------------------------------------------|
| (II) chromate(VI)(2-)    | PbCrO <sub>4</sub>                                                 | 323.2  | 6.12                | 844                                                        | d           | i aq; s dil HNO <sub>3</sub> , alkalis                                                                      |
| (II) fluoride            | PbF <sub>2</sub>                                                   | 245.2  | 8.445               | 830                                                        | 1297        | 0.064 <sup>20</sup> aq                                                                                      |
| (IV) fluoride            | PbF <sub>4</sub>                                                   | 283.2  | 6.7                 | ≈ 600                                                      |             | hyd aq                                                                                                      |
| (II) formate             | Pb(CHO <sub>2</sub> ) <sub>2</sub>                                 | 297.2  | 4.63                | d 190                                                      |             | 1.6 g/100 mL <sup>20</sup> aq                                                                               |
| (II) hydrogen arsenate   | PbHAsO <sub>4</sub>                                                | 347.1  | 5.94                | d 280 to<br>Pb <sub>2</sub> As <sub>2</sub> O <sub>7</sub> |             | s HNO <sub>3</sub> , alkalis                                                                                |
| (II) hydroxide           | Pb(OH) <sub>2</sub>                                                | 241.2  | 7.59                | d 145                                                      |             | 0.016 <sup>20</sup> aq; s acids, alkalis                                                                    |
| (II) iodide              | PbI <sub>2</sub>                                                   | 461.0  | 6.16                | 410                                                        | 872         | 0.063 <sup>20</sup> aq; s KI, Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> , alkalis                       |
| (II) molybdate(VI)(2-)   | PbMoO                                                              | 367.1  | 6.7                 | 1065                                                       |             | s acids, alkalis                                                                                            |
| (II) nitrate             | Pb(NO <sub>3</sub> ) <sub>2</sub>                                  | 331.2  | 4.53                | 470                                                        |             | g/100 mL: 56 <sup>20</sup> aq, 1.3 MeOH                                                                     |
| (II) oleate              | Pb(C <sub>18</sub> H <sub>33</sub> O <sub>2</sub> ) <sub>2</sub>   | 770.1  |                     |                                                            |             | s alc, bz, eth                                                                                              |
| (II) oxalate             | PbC <sub>2</sub> O <sub>4</sub>                                    | 295.2  | 5.28                | d 300                                                      |             | s acids, alkalis                                                                                            |
| (II) oxide (litharge)    | PbO                                                                | 223.2  | 9.35 (red)          | 886                                                        | 1472 d      | 0.0017 <sup>20</sup> aq; s HNO <sub>3</sub>                                                                 |
| (IV) oxide               | PbO <sub>2</sub>                                                   | 239.2  | 9.64                | d 290, Pb <sub>3</sub> O <sub>4</sub>                      | d 595, PbO  | s HCl, dil HNO <sub>3</sub> + H <sub>2</sub> O <sub>23</sub> , H <sub>2</sub> C <sub>2</sub> O <sub>4</sub> |
| (II,IV) oxide (red lead) | Pb <sub>3</sub> O <sub>4</sub>                                     | 685.6  | 8.92                | d 595 → PbO                                                |             | s HNO <sub>3</sub> , hot HCl                                                                                |
| (II) phosphate           | Pb <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>                    | 811.5  | 7.0                 | 1014                                                       |             | s HNO <sub>3</sub> , alkalis                                                                                |
| (II) selenide            | PbSe                                                               | 286.2  | 8.15                | 1078                                                       |             | s HNO <sub>3</sub>                                                                                          |
| (II) silicate(2-)        | PbSiO <sub>3</sub>                                                 | 283.3  | 6.5                 | 764                                                        |             | s acids                                                                                                     |
| (II) silicate(4-)        | Pb <sub>2</sub> SiO <sub>4</sub>                                   | 506.5  | 7.60                | 743                                                        |             |                                                                                                             |
| (II) stearate            | Pb(C <sub>18</sub> H <sub>35</sub> O <sub>2</sub> ) <sub>2</sub>   | 774.2  | 1.4                 | ≈ 125                                                      |             | 0.05 <sup>35</sup> aq; s hot alc                                                                            |
| (II) sulfate             | PbSO <sub>4</sub>                                                  | 303.3  | 6.29                | 1170                                                       |             | 0.00425 aq; s NaOH                                                                                          |
| (II) sulfide             | PbS                                                                | 239.3  | 7.60                | 1118                                                       | 1300 subl   | 0.0006 <sup>18</sup> aq; s HNO <sub>3</sub> , hot dil HCl                                                   |
| (II) telluride           | PbTe                                                               | 334.8  | 8.16                | 924                                                        |             | i acids and alkalis                                                                                         |
| tetraethyl               | Pb(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub>                    | 323.45 | 1.653               | - 137                                                      | ≈ 200       | i aq; s bz, hydrocarbons                                                                                    |
| tetramethyl              | Pb(CH <sub>3</sub> ) <sub>4</sub>                                  | 267.35 | 1.995               | - 30.2                                                     | 110         | s hydrocarbons                                                                                              |
| (II) thiocyanate         | Pb(SCN) <sub>2</sub>                                               | 323.4  | 3.82                | d 190                                                      |             | 0.44 <sup>18</sup> aq, s HNO <sub>3</sub> , NaOH                                                            |
| Lithium                  | Li                                                                 | 6.941  | 0.534 <sup>20</sup> | 180.54                                                     | 1341        | d aq to LiOH                                                                                                |
| acetate 2-water          | LiC <sub>2</sub> H <sub>3</sub> O <sub>2</sub> · 2H <sub>2</sub> O | 102.02 | 1.3                 | 58                                                         | d           | 63 g/100 mL <sup>20</sup> aq; v s alc                                                                       |
| aluminate(1-)            | LiAlO <sub>2</sub>                                                 | 65.92  | 2.554               | 1700                                                       |             |                                                                                                             |
| amide                    | LiNH <sub>2</sub>                                                  | 22.96  | 1.178               | 380                                                        | d 450 vacuo | d aq (→ LiOH + NH <sub>3</sub> ); i bz, eth                                                                 |
| benzoate                 | LiC <sub>7</sub> H <sub>5</sub> O <sub>2</sub>                     | 128.06 |                     | > 300                                                      |             | g/100 mL: 33 aq; 7.7 alc                                                                                    |
| borate(1-)               | LiBO <sub>2</sub>                                                  | 49.75  | 2.18                | 849                                                        | 1719        | 2.7 g/100 mL <sup>20</sup> aq; i alc                                                                        |
| borohydride              | Li[BH <sub>4</sub> ]                                               | 21.78  | 0.66                | 268                                                        | d 380       | s aq, eth, THF, aliphatic amines                                                                            |
| bromate                  | LiBrO <sub>3</sub>                                                 | 134.85 | 3.62                |                                                            |             | 179 g/100 mL <sup>20</sup> aq                                                                               |
| bromide                  | LiBr                                                               | 86.84  | 3.464               | 552                                                        | 1289        | 164 g/100 mL aq; s alc, eth                                                                                 |
| carbonate                | Li <sub>2</sub> CO <sub>3</sub>                                    | 73.89  | 2.11                | 720                                                        | d 1300      | 1.3 g/100 mL <sup>20</sup> aq; i alc; s acids                                                               |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

|      | Name                         | Formula                                                                          | Formula weight | Density                         | Melting point,               | Boiling point,                   | Solubility in<br>100 parts solvent               |
|------|------------------------------|----------------------------------------------------------------------------------|----------------|---------------------------------|------------------------------|----------------------------------|--------------------------------------------------|
|      |                              |                                                                                  |                |                                 | °C                           | °C                               |                                                  |
| 3.36 | Lithium ( <i>continued</i> ) |                                                                                  |                |                                 |                              |                                  |                                                  |
|      | chloride                     | LiCl                                                                             | 42.39          | 2.07                            | 613                          | 1360                             | 77 g/100 mL <sup>20</sup> aq; s alc, acet        |
|      | chromate(VI)(2−) 2-water     | Li <sub>2</sub> CrO <sub>4</sub> · 2H <sub>2</sub> O                             | 165.91         | 2.15                            | anhyd 75                     |                                  | 142 g/100 mL <sup>18</sup> aq; s EtOH            |
|      | citrate 4-water              | Li <sub>3</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> · 4H <sub>2</sub> O | 281.98         |                                 | anhyd 105                    |                                  | 61 g/100 mL <sup>15</sup> aq; sl s alc           |
|      | fluoride                     | LiF                                                                              | 25.94          | 2.640                           | 848                          | 1681                             | 0.13 <sup>25</sup> aq; s acids                   |
|      | hexafluoroaluminate(3−)      | Li <sub>3</sub> [AlF <sub>6</sub> ]                                              | 161.79         |                                 | 1012                         |                                  |                                                  |
|      | hydride                      | LiH                                                                              | 7.95           | 0.76–0.77                       | 680                          | d 950                            | no solvent known; flammable                      |
|      | hydride- <i>d</i>            | Li <sup>2</sup> H or LiD                                                         | 8.96           | 0.881                           | 686                          |                                  |                                                  |
|      | hydroxide                    | LiOH                                                                             | 23.95          | 1.45                            | 471.2                        | 1626                             | 12.4 g/100 mL <sup>20</sup> aq; sl s alc         |
|      | iodate                       | LiIO <sub>3</sub>                                                                | 181.84         | 4.502                           | 450                          |                                  | 66 g/100 mL aq; in alc                           |
|      | iodide                       | LiI                                                                              | 133.84         | 4.061                           | 469                          | 1174                             | 165 g/100 mL <sup>20</sup> aq & alc; v s acet    |
|      | nitrate                      | LiNO <sub>3</sub>                                                                | 68.95          | 2.38                            | ~ 255                        |                                  | 50 g/100 mL <sup>20</sup> aq; s alc              |
|      | nitride                      | Li <sub>3</sub> N                                                                | 34.83          | 1.27                            | 813                          |                                  | d aq                                             |
|      | oxide                        | Li <sub>2</sub> O                                                                | 29.88          | 2.013                           | 1570                         | 2563                             | forms LiOH in aq                                 |
|      | perchlorate                  | LiClO <sub>4</sub>                                                               | 106.39         | 2.43                            | 236                          | d ~ 400<br>LiCl + O <sub>2</sub> | 47.4 g/100 mL <sup>25</sup> aq; v s organic solv |
|      | peroxide                     | Li <sub>2</sub> O <sub>2</sub>                                                   | 45.88          | 2.31                            | d > 195 to Li <sub>2</sub> O |                                  |                                                  |
|      | silicate(2−)                 | Li <sub>2</sub> SiO <sub>3</sub>                                                 | 89.97          | 2.52 <sub>4</sub> <sup>25</sup> | 1201                         |                                  | d dil HCl                                        |
|      | sulfate                      | Li <sub>2</sub> SO <sub>4</sub>                                                  | 109.95         | 2.22                            | 859                          |                                  | 34.5 g/100 mL <sup>20</sup> aq; i alc            |
|      | tetraborate(2−)              | Li <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                                    | 169.12         |                                 | 917                          |                                  | sl s aq                                          |
|      | tetrahydridoaluminate        | Li[AlH <sub>4</sub> ]                                                            | 37.95          | 0.917                           | d 137                        |                                  | d aq, alc; g/100 mL: 30 eth, 13 THF; flammable   |
|      | tetrahydridoborate           | LiBH <sub>4</sub>                                                                | 21.79          | 0.666                           | 268                          | d 380                            | s aq pH > 7; s eth, THF                          |
|      | Lutetium                     | Lu                                                                               | 174.967        | 9.841                           | 1663                         | 3402                             | s acids                                          |
|      | chloride                     | LuCl <sub>3</sub>                                                                | 281.33         | 3.98                            | 892                          | subl > 750                       | s aq                                             |
|      | sulfate 8-water              | Lu <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O              | 782.25         |                                 |                              |                                  | 42.3 g/100 mL <sup>20</sup> aq                   |
|      | Magnesium                    | Mg                                                                               | 24.305         | 1.738 <sup>20</sup>             | 651                          | 1100                             | i aq; s dilute acids                             |
|      | acetate                      | Mg(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub>                   | 142.00         | 1.42                            | 323 d                        |                                  | 53.4 g/100 mL <sup>20</sup> aq; v s alc          |
|      | aluminate(2−)                | MgAl <sub>2</sub> O <sub>4</sub>                                                 | 142.25         | 3.6                             | 2135                         |                                  | v sl s HCl                                       |
|      | amide                        | Mg(NH <sub>2</sub> ) <sub>2</sub>                                                | 56.35          | 1.39 <sub>4</sub> <sup>25</sup> | ign in air                   |                                  | d viol water giving NH <sub>3</sub>              |
|      | borate(1−) 8-water           | Mg(BO <sub>2</sub> ) <sub>2</sub> · 8H <sub>2</sub> O                            | 254.04         | 2.30                            |                              |                                  | sl s aq; s acids                                 |
|      | bromide                      | MgBr <sub>2</sub>                                                                | 184.11         | 3.722                           | 711 d                        | 1158                             | 101 g/100 mL <sup>20</sup> aq                    |

|                            |                                                                                    |         |                     |                          |            |                                                                       |
|----------------------------|------------------------------------------------------------------------------------|---------|---------------------|--------------------------|------------|-----------------------------------------------------------------------|
| carbonate                  | MgCO <sub>3</sub>                                                                  | 84.31   | 3.05                | 990                      |            | 0.01 aq; s acids                                                      |
| chloride                   | MgCl <sub>2</sub>                                                                  | 95.21   | 2.33                | 714                      | 1412       | 54.6 g/100 mL <sup>20</sup> aq                                        |
| fluoride                   | MgF <sub>2</sub>                                                                   | 62.30   | 3.148               | 1263                     | 2270       | 0.013 <sup>25</sup> aq; s HNO <sub>3</sub>                            |
| ( <i>di</i> -) germanide   | Mg <sub>2</sub> Ge                                                                 | 121.22  | 3.09                | 1115                     |            |                                                                       |
| hexafluorosilicate 6-water | Mg[SiF <sub>6</sub> ] · 6H <sub>2</sub> O                                          | 274.47  | 1.788               | — SiF <sub>4</sub> , 120 |            | 51 g/100 mL <sup>20</sup> aq; i alc                                   |
| hydride                    | MgH <sub>2</sub>                                                                   | 26.32   | 1.45                | d 200 vacuo              | ign in air | d aq and alc violently                                                |
| hydrogen phosphate 3-water | MgHPO <sub>4</sub> · 3H <sub>2</sub> O                                             | 174.33  | 2.13 <sup>15</sup>  | anhyd 205                | d 550      | sl s aq; s acids                                                      |
| hydroxide                  | Mg(OH) <sub>2</sub>                                                                | 58.32   | 2.36                | 350 d                    |            | 0.00125 aq; s acids                                                   |
| iodide                     | MgI <sub>2</sub>                                                                   | 278.12  | 4.43                | 634                      | 0          | 140 g/100 mL <sup>20</sup> aq; s alc                                  |
| lactate 3-water            | MgC <sub>6</sub> H <sub>10</sub> O <sub>6</sub> · 3H <sub>2</sub> O                | 256.51  |                     |                          |            | 4 g/100 mL aq; sl s alc                                               |
| mandelate                  | MgC <sub>16</sub> H <sub>14</sub> O <sub>6</sub>                                   | 326.59  |                     |                          |            | 0.004 <sup>100</sup> aq; i alc                                        |
| nitrate                    | Mg(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                              | 256.41  | 1.464               | 95                       | d 129      | 120 g/100 mL <sup>20</sup> aq; v s alc                                |
| nitride                    | Mg <sub>3</sub> N <sub>2</sub>                                                     | 100.93  | 2.712               | d 270                    |            | d aq; s acids                                                         |
| oleate                     | Mg(C <sub>18</sub> H <sub>33</sub> O <sub>2</sub> ) <sub>2</sub>                   | 587.22  |                     |                          |            | sl s alc, eth, PE                                                     |
| oxide                      | MgO                                                                                | 40.30   | 3.65–3.75           | 2800                     | 3600       | i aq, alc; s acids                                                    |
| perchlorate                | Mg(ClO <sub>4</sub> ) <sub>2</sub>                                                 | 223.21  | 2.21                | d > 251                  |            | g/100 mL <sup>25</sup> ; 73 aq, 18 EtOH, 44.6 BuOH, 54 EtOAc, 32 acet |
| permanganate               | Mg(MnO <sub>4</sub> ) <sub>2</sub>                                                 | 262.19  |                     |                          |            | v s aq                                                                |
| peroxide                   | MgO <sub>2</sub>                                                                   | 56.30   | ≈ 3.0               | d 100                    |            | s acids                                                               |
| peroxoborate 7-water       | Mg(BO <sub>3</sub> ) <sub>2</sub> · 7H <sub>2</sub> O                              | 268.09  |                     |                          |            | sl s aq d; s dilute acids                                             |
| phosphate 5-water          | Mg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> · 5H <sub>2</sub> O                | 352.96  | 1.64 <sup>15</sup>  | anhyd ~ 400              |            | 0.02 aq; s acids                                                      |
| silicate(2–)               | MgSiO <sub>3</sub>                                                                 | 100.39  | 3.192 <sup>25</sup> | d 1557                   |            | i aq; v sl s HF                                                       |
| silicate(4–)               | Mg <sub>2</sub> SiO <sub>4</sub>                                                   | 140.69  | 3.21                | 1898                     |            | i aq; d hot HCl                                                       |
| ( <i>di</i> -) silicide    | Mg <sub>2</sub> Si                                                                 | 76.70   | 2.0                 | 1100                     |            | d aq, HCl                                                             |
| ( <i>di</i> -) stannide    | Mg <sub>2</sub> Sn                                                                 | 167.32  | 3.60                | 778                      |            | s aq, HCl                                                             |
| sulfate 7-water            | MgSO <sub>4</sub> · 7H <sub>2</sub> O                                              | 246.47  | 1.67                | anhyd 250                |            | 27.2 g/100 mL aq; sl s alc                                            |
| sulfite 6-water            | MgSO <sub>3</sub> · 6H <sub>2</sub> O                                              | 212.46  | 1.725               | anhyd 200                | mp: 2227   | 0.66 <sup>25</sup> aq                                                 |
| tungstate(VI)(2–)          | MgWO <sub>4</sub>                                                                  | 272.14  | 6.89                |                          |            | i aq; d acids                                                         |
| Manganese                  | Mn                                                                                 | 54.9380 | 7.21 <sup>20</sup>  | 1244 fctetr              | 2095       | d aq; s acids                                                         |
| acetate 4-water            | Mn(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 4H <sub>2</sub> O | 245.09  | 1.589               | 80                       |            | 38 g/100 mL <sup>50</sup> aq; v s alc                                 |
| bromide                    | MnBr <sub>2</sub>                                                                  | 214.75  | 4.39                | 698                      | 1027       | 147 g/100 mL <sup>20</sup> aq; s alc                                  |
| ( <i>tri</i> -) carbide    | Mn <sub>3</sub> C                                                                  | 176.83  | 6.89                | 1520                     |            | d aq; s acid                                                          |
| carbonate                  | MnCO <sub>3</sub>                                                                  | 114.95  | 3.125               | d > 200                  |            | 0.0065 <sup>25</sup> aq; s acids                                      |
| chloride                   | MnCl <sub>2</sub>                                                                  | 125.84  | 2.977               | 650                      | 1210       | 74 g/100 mL <sup>20</sup> aq; s alc, pyr; i eth                       |
| chloride 4-water           | MnCl <sub>2</sub> · 4H <sub>2</sub> O                                              | 187.91  | 2.01                | 97.5                     | anhyd 198  | 143 g/100 mL aq; s alc; i eth                                         |
| decarbonyl                 | Mn <sub>2</sub> (CO) <sub>10</sub>                                                 | 389.98  | 1.75                | d 110                    |            | i aq; s organic solvents                                              |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                           | Formula                                                             | Formula weight | Density | Melting point,<br>°C   | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                             |
|--------------------------------|---------------------------------------------------------------------|----------------|---------|------------------------|----------------------|--------------------------------------------------------------------------------|
| Manganese ( <i>continued</i> ) |                                                                     |                |         |                        |                      |                                                                                |
| diphosphate                    | Mn <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                       | 283.82         | 3.707   | 1196                   |                      | i aq; s acid                                                                   |
| (II) fluoride                  | MnF <sub>2</sub>                                                    | 92.93          | 3.98    | 930                    | 1820                 | 0.66 <sup>40</sup> aq; s HF, conc HCl                                          |
| (III) fluoride                 | MnF <sub>3</sub>                                                    | 111.93         | 3.54    | d >600                 |                      | hyd aq; s acid                                                                 |
| hydroxide                      | Mn(OH) <sub>2</sub>                                                 | 88.95          | 3.258   | d                      |                      | 0.002 <sup>18</sup> aq; s acids                                                |
| iodide                         | MnI <sub>2</sub>                                                    | 308.75         | 5.04    | 638                    | 1017                 | s aq                                                                           |
| nitrate 6-water                | Mn(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O               | 287.04         | 1.8     | 25.8                   |                      | v s aq, alc                                                                    |
| (II) oxide                     | MnO                                                                 | 70.94          | 5.37    | 1840                   |                      | i aq; s acids                                                                  |
| (III) oxide                    | Mn <sub>2</sub> O <sub>3</sub>                                      | 157.87         | 4.89    | 877 d                  |                      | i aq; s HCl giving off Cl <sub>2</sub>                                         |
| (IV) oxide                     | MnO <sub>2</sub>                                                    | 86.94          | 5.08    | — O <sub>2</sub> , 530 |                      | s HCl; i HNO <sub>3</sub> , cold H <sub>2</sub> SO <sub>4</sub>                |
| (II,IV) oxide                  | Mn <sub>3</sub> O <sub>4</sub>                                      | 228.81         | 4.84    | 1567                   |                      | i aq; s HCl                                                                    |
| (VII) oxide                    | Mn <sub>2</sub> O <sub>7</sub>                                      | 221.87         | 2.396   | ca. — 20               | ca. 25               | explodes 85; v s aq                                                            |
| phosphinate hydrate            | Mn(PH <sub>2</sub> O <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O | 202.93         |         | d to PH <sub>3</sub>   |                      | 15 g/100 mL aq; i alc                                                          |
| silicate, meta-                | MnSiO <sub>3</sub>                                                  | 131.02         | 3.48    | 1290                   |                      | i aq, HCl                                                                      |
| sulfate                        | MnSO <sub>4</sub>                                                   | 151.00         | 3.25    | 700                    | d 850                | 52 g/100 mL aq; i alc                                                          |
| sulfate hydrate                | MnSO <sub>4</sub> · H <sub>2</sub> O                                | 169.02         | 2.95    | anhyd 400–450          |                      | 70 g/100 mL <sup>20</sup> aq                                                   |
| sulfate 7-water                | MnSO <sub>4</sub> · 7H <sub>2</sub> O                               | 277.11         | 2.09    | anhyd 280              |                      | 115 g/100 mL <sup>20</sup> aq                                                  |
| sulfide                        | MnS                                                                 | 87.00          | 3.99    | 1610                   |                      | 0.0006 <sup>18</sup> aq; s acids                                               |
| titanate(IV)(2–)               | Mn <sub>2</sub> TiO <sub>4</sub>                                    | 150.84         | 4.54    | 1360                   |                      |                                                                                |
| Mercury                        | Hg                                                                  | 200.59         | 13.534  | – 38.83                | 356.7                | i aq; s HNO <sub>3</sub> , hot conc H <sub>2</sub> SO <sub>4</sub>             |
| (II) acetate                   | Hg(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub>      | 318.68         | 3.28    | 178–180 d              |                      | g/100 mL: 40 <sup>10</sup> aq, 7.5 <sup>15</sup> MeOH                          |
| (II) benzoate                  | Hg(C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> ) <sub>2</sub>      | 424.83         |         | 165                    |                      | v s NaCl soln; sl s alc                                                        |
| (I) bromide                    | Hg <sub>2</sub> Br <sub>2</sub>                                     | 560.99         | 7.307   | subl 393 d             |                      | i aq, alc, eth; d hot HCl                                                      |
| (II) bromide                   | HgBr <sub>2</sub>                                                   | 360.40         | 6.05    | 237                    | 322 subl             | g/100 mL: 0.56 <sup>20</sup> aq; 20 <sup>25</sup> alc; v s HCl, HBr            |
| (I) chloride                   | Hg <sub>2</sub> Cl <sub>2</sub>                                     | 472.09         | 7.16    | subl 382               | d without melting    | s aqua regia; i aq, alc, eth                                                   |
| (II) chloride                  | HgCl <sub>2</sub>                                                   | 271.50         | 5.4     | 277                    | 304                  | g/100 mL <sup>20</sup> : 7.15 aq, 26 alc, 4 eth 8.3 glyc, 0.5 bz; s HOAc, EtAc |
| (II) cyanide                   | Hg(CN) <sub>2</sub>                                                 | 252.63         | 4.00    | d 320                  |                      | g/100 mL <sup>20</sup> : 9.3 aq, 25 MeOH, 8 EtOH                               |
| (I) fluoride                   | Hg <sub>2</sub> F <sub>2</sub>                                      | 439.18         | 8.73    | >570 d                 |                      | hydrolyses in water                                                            |



|                           |                                                                                    |          |                         |           |                      |                                                                                        |
|---------------------------|------------------------------------------------------------------------------------|----------|-------------------------|-----------|----------------------|----------------------------------------------------------------------------------------|
| (II) fluoride             | HgF <sub>2</sub>                                                                   | 238.59   | 8.95                    | d 645     | d >650               | hyd aq; s HF                                                                           |
| (II) fulminate            | Hg(ONC) <sub>2</sub>                                                               | 284.62   | 4.42                    | explodes  |                      | sl s aq; s alc; dangerously flammable                                                  |
| (I) iodide                | Hg <sub>2</sub> I <sub>2</sub>                                                     | 654.99   | 7.70                    | 290 d     | subl 140             | i aq, alc, eth; s KI                                                                   |
| (II) iodide               | HgI <sub>2</sub>                                                                   | 454.40   | 6.28                    | 259       | 350 subl             | g/100 mL: 0.006 <sup>25</sup> aq, 0.8 alc, 0.8 eth, 1.7 acet                           |
| (I) nitrate 2-water       | Hg <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> · 2H <sub>2</sub> O                | 561.22   | 4.79                    | 70 d      |                      | hyd aq; s HNO <sub>3</sub>                                                             |
| (II) nitrate              | Hg(NO <sub>3</sub> ) <sub>2</sub>                                                  | 324.60   | 4.3                     | 79        | d                    | v s aq; s acet                                                                         |
| (I) oxide                 | Hg <sub>2</sub> O                                                                  | 417.18   | 9.8                     | d 100     |                      | i aq; s HNO <sub>3</sub>                                                               |
| (II) oxide                | HgO                                                                                | 216.59   | 11.14                   | d 500     |                      | 0.005 <sup>25</sup> aq; s dil HCl, HNO <sub>3</sub> , I <sup>-</sup> , CN <sup>-</sup> |
| (I) sulfate               | Hg <sub>2</sub> SO <sub>4</sub>                                                    | 497.24   | 7.56                    | d         |                      | 0.06 <sup>25</sup> aq; s HNO <sub>3</sub>                                              |
| (II) sulfate              | HgSO <sub>4</sub>                                                                  | 296.65   | 6.47                    | d         |                      | s acid                                                                                 |
| (II) sulfide (cinnabar)   | HgS                                                                                | 232.66   | 8.17                    | subl 583  | → blk HgO, 386       | i aq; s aqua regia                                                                     |
| (II) thiocyanate          | Hg(SCN) <sub>2</sub>                                                               | 316.76   | 3.71                    | d 165     |                      | 0.063 <sup>25</sup> aq; s HCl                                                          |
| Molybdenum                | Mo                                                                                 | 95.94    | 10.28                   | 2622      | 4825                 | s hot H <sub>2</sub> SO <sub>4</sub> , HNO <sub>3</sub> , fused KNO <sub>3</sub>       |
| (III) bromide             | MoBr <sub>3</sub>                                                                  | 335.65   | 4.89                    | subl 977  |                      | d alkalis                                                                              |
| (IV) chloride             | MoCl <sub>4</sub>                                                                  | 237.75   |                         | 317       | 407                  | s conc acids                                                                           |
| (V) chloride              | MoCl <sub>5</sub>                                                                  | 273.19   | 2.928                   | 194       | 268                  | s conc acids, dry eth, dry alc                                                         |
| (VI) fluoride             | MoF <sub>6</sub>                                                                   | 209.93   | 2.54                    | 17.6      | 35.0                 | hyd aq; s alkalis; 31 g/100 g HF                                                       |
| hexacarbonyl              | Mo(CO) <sub>6</sub>                                                                | 264.00   | 1.96                    | 150 d     | subl                 | s bz                                                                                   |
| (IV) oxide                | MoO <sub>2</sub>                                                                   | 127.94   | 6.47                    | d ≈1100   |                      | i aq                                                                                   |
| (VI) oxide                | MoO <sub>3</sub>                                                                   | 143.94   | 4.696 <sup>26</sup>     | 801       | 1155                 | 0.05 <sup>28</sup> aq; s conc mineral acids, alk                                       |
| (III) sulfide             | Mo <sub>2</sub> S <sub>3</sub>                                                     | 288.07   | 5.91 <sup>15</sup>      | 1807      | d 1867               | d hot HNO <sub>3</sub>                                                                 |
| (IV) sulfide              | MoS <sub>2</sub>                                                                   | 160.07   | 5.06 <sup>15</sup>      | 2375      | subl 450             | s aqua regia                                                                           |
| Neodymium                 | Nd                                                                                 | 144.24   | 7.01                    | 1024      | 3074                 | s hot aq, acids                                                                        |
| chloride                  | NdCl <sub>3</sub>                                                                  | 250.60   | 4.134                   | 760       | 1600                 | 98 g/100 mL <sup>20</sup> aq; s alc                                                    |
| oxide                     | Nd <sub>2</sub> O <sub>3</sub>                                                     | 336.48   | 7.28                    | 1900      |                      | s dilute acids                                                                         |
| sulfate 8-water           | Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O                | 720.79   | 2.85                    | d 700–800 |                      | 8.87 g/100 mL <sup>20</sup> aq                                                         |
| Neon                      | Ne                                                                                 | 20.180   | 0.8999 g/L <sup>0</sup> | – 248.67  | – 246.05             | 1.05 mL <sup>20</sup> aq                                                               |
| Neptunium                 | Np                                                                                 | 237.0482 | 20.2                    | 644       | >3900                | s HCl                                                                                  |
| (IV) oxide                | NpO <sub>2</sub>                                                                   | 269      | 11.1                    | 2547      |                      |                                                                                        |
| Nickel                    | Ni                                                                                 | 58.69    | 8.908 <sup>20</sup>     | 1453      | 2884                 | i aq; s HNO <sub>3</sub>                                                               |
| acetate 4-water           | Ni(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 4H <sub>2</sub> O | 248.86   | 1.744                   | d         |                      | 16 g/100 mL aq; s alc                                                                  |
| acetylacetonate           | Ni(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub>                     | 256.91   | 1.455 <sup>17</sup>     | 230       | 235 <sup>11atm</sup> | s aq, alc, bz, chl; i eth                                                              |
| bromide                   | NiBr <sub>2</sub>                                                                  | 218.50   | 5.098                   | 963       | subl                 | 100 g/100 mL <sup>20</sup> aq                                                          |
| carbonate hydroxide (1/2) | NiCO <sub>3</sub> · 2Ni(OH) <sub>2</sub>                                           | 304.12   | 2.6                     |           |                      | s dilute acids                                                                         |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

|          | Name                        | Formula                                                                        | Formula weight | Density                 | Melting point,          | Boiling point, | Solubility in<br>100 parts solvent                                  |
|----------|-----------------------------|--------------------------------------------------------------------------------|----------------|-------------------------|-------------------------|----------------|---------------------------------------------------------------------|
|          |                             |                                                                                |                |                         | °C                      | °C             |                                                                     |
| 3.40     | Nickel ( <i>continued</i> ) |                                                                                |                |                         |                         |                |                                                                     |
|          | carbonyl                    | Ni(CO) <sub>4</sub>                                                            | 170.73         | 1.31                    | − 19.3                  | 43 (expl 60)   | s EtOH, bz, acet                                                    |
|          | chloride                    | NiCl                                                                           | 129.60         | 3.51                    | 1009                    | subl 973       | 61 g/100 mL <sup>20</sup> aq                                        |
|          | chloride 6-water            | NiCl <sub>2</sub> · 6H <sub>2</sub> O                                          | 237.69         |                         |                         |                | 100 g/100 mL <sup>20</sup> aq; s alc                                |
|          | cyanide 4-water             | Ni(CN) <sub>2</sub> · 4H <sub>2</sub> O                                        | 182.79         |                         | anhyd 400               |                | 0.006 <sup>18</sup> aq; s KCN, NH <sub>4</sub> OH                   |
|          | dimethylglyoxime            | Ni(HC <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub> | 288.92         |                         | subl 250                |                | i aq; s abs alc, dilute acids                                       |
|          | ( <i>tri</i> -) disulfide   | Ni <sub>3</sub> S <sub>2</sub>                                                 | 240.21         | 5.87                    | 790                     | d 2967         | s HNO <sub>3</sub>                                                  |
|          | fluoride                    | NiF <sub>2</sub>                                                               | 96.69          | 4.72                    | 1450                    | 1740           | 4 g/100 mL <sup>20</sup> aq; i alc, eth                             |
|          | formate 2-water             | Ni(CHO <sub>2</sub> ) <sub>2</sub> · 2H <sub>2</sub> O                         | 184.78         | 2.154 <sup>20</sup>     | anhyd 130               | d 180–200      | s aq; i alc                                                         |
|          | nitrate 6-water             | Ni(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                          | 290.81         | 2.05                    | 56.7                    | 136.7          | 150 g/100 mL <sup>20</sup> aq                                       |
|          | (II) oxide                  | NiO                                                                            | 74.71          | 7.45                    | 2000                    |                | s acids                                                             |
|          | (III) oxide                 | Ni <sub>2</sub> O <sub>3</sub>                                                 | 165.42         | 4.83                    | − O <sub>2</sub> , 600  |                | s hot HCl, HNO <sub>3</sub> , H <sub>2</sub> SO <sub>4</sub>        |
|          | sulfate                     | NiSO <sub>4</sub>                                                              | 154.78         | 3.68                    | − SO <sub>3</sub> , 840 |                | 29 g/100 mL <sup>9</sup> aq                                         |
|          | sulfate 6-water             | NiSO <sub>4</sub> · 6H <sub>2</sub> O                                          | 262.86         | 2.07                    | anhyd 280               |                | 40 g/100 mL <sup>20</sup> aq                                        |
|          | sulfide                     | NiS                                                                            | 90.77          | 5.3–5.6                 | 976                     | d 2047         | s HNO <sub>3</sub> , KHS                                            |
|          | tetracarbonyl               | Ni(CO) <sub>4</sub>                                                            | 170.74         | 1.3185 <sup>17</sup>    | − 19.3                  | 42.3           | explodes 63; FP − 4; s organic sol-<br>vents                        |
|          | Niobium                     | Nb                                                                             | 92.9064        | 8.57 <sup>20</sup>      | 2468                    | 4860           | s fused alkali hydroxides                                           |
|          | (V) chloride                | NbCl <sub>5</sub>                                                              | 270.20         | 2.75                    | 206                     | 247.0          | s HCl, CCl <sub>4</sub>                                             |
|          | (V) fluoride                | NbF <sub>5</sub>                                                               | 187.91         | 2.696 <sup>80</sup>     | 80.0                    | 234.9          | hyd aq, alc; sl s CS <sub>2</sub> , CCl <sub>4</sub>                |
|          | (V) oxide                   | Nb <sub>2</sub> O <sub>5</sub>                                                 | 265.82         | 4.55                    | 1512                    |                | s HF, hot H <sub>2</sub> SO <sub>4</sub>                            |
| Nitrogen |                             | N <sub>2</sub>                                                                 | 28.0341        | 1.165 g/L <sup>20</sup> | − 210.01                | − 195.79       | mL/100 mL: 1.6 <sup>20</sup> aq, 0.112 alc                          |
|          |                             | <sup>15</sup> N <sub>2</sub>                                                   | 30.01          | 1.25 g/L <sup>20</sup>  | − 209.952               | − 195.73       |                                                                     |
|          | (I) oxide                   | N <sub>2</sub> O                                                               | 44.02          | 1.843 g/L <sup>20</sup> | − 90.81                 | − 88.46        | 130 <sup>0</sup> mL aq; s alc, eth                                  |
|          | (II) oxide                  | NO                                                                             | 30.01          | 1.249 g/L <sup>20</sup> | − 163.64                | − 151.76       | 4.6 mL/100 mL <sup>20</sup> aq                                      |
|          | (III) oxide                 | N <sub>2</sub> O <sub>3</sub>                                                  | 76.02          | 1.447 g/L <sup>2</sup>  | − 100.7                 | 2              | s eth                                                               |
|          | (IV) oxide dimer            | N <sub>2</sub> O <sub>4</sub>                                                  | 92.02          | 1.448 <sup>20</sup>     | − 9.3                   | 21.15 d        | s conc HNO <sub>3</sub> , conc H <sub>2</sub> SO <sub>4</sub> , chl |
|          | (V) oxide                   | N <sub>2</sub> O <sub>5</sub>                                                  | 108.01         | 2.05                    | 30                      | 47.0           | v s chl; s CCl <sub>4</sub>                                         |
|          | selenide                    | N <sub>4</sub> Se <sub>4</sub>                                                 | 371.87         | 4.2                     | explosive               |                | sl s bz, CS <sub>2</sub>                                            |
|          | sulfide                     | N <sub>4</sub> S <sub>4</sub>                                                  | 184.28         | 2.24 <sup>18</sup>      | 180                     | 185            | s organic solvents                                                  |
|          | trichloride                 | NCl <sub>3</sub>                                                               | 120.37         | 1.653 <sup>20</sup>     | − 27                    | 71             | i aq; s bz, CS <sub>2</sub> , CCl <sub>4</sub>                      |
|          | trifluoride                 | NF <sub>3</sub>                                                                | 70.01          | 2.96 g/L <sup>20</sup>  | − 208.5                 | − 129.06       |                                                                     |

|                               |                                                                |          |                                  |                            |                          |                                                                                      |
|-------------------------------|----------------------------------------------------------------|----------|----------------------------------|----------------------------|--------------------------|--------------------------------------------------------------------------------------|
| Nitrosyl chloride             | NOCl                                                           | 65.47    | 1.592 <sup>-5</sup>              | − 61.5                     | − 5.5                    | hyd aq; s fuming H <sub>2</sub> SO <sub>4</sub>                                      |
| fluoride                      | NOF                                                            | 49.01    | 2.788 g/L <sup>20</sup>          | − 132.5                    | − 59.9                   | hyd aq                                                                               |
| hydrogen sulfate              | NOHSO <sub>4</sub>                                             | 127.08   |                                  | d 73.5                     |                          | d aq; s H <sub>2</sub> SO <sub>4</sub>                                               |
| tetrafluoroborate             | NO[BF <sub>4</sub> ]                                           | 116.83   | 2.185 <sup>25</sup> <sub>4</sub> | subl 250 <sup>0.01mm</sup> |                          | d aq                                                                                 |
| Nitryl chloride               | NO <sub>2</sub> Cl                                             | 81.46    | 2.81 g/L <sup>100</sup>          | − 145                      | − 14.3                   | d aq                                                                                 |
| fluoride                      | NO <sub>2</sub> F                                              | 65.00    | 2.7 g/L <sup>20</sup>            | − 166.0                    | − 72.4                   | d aq                                                                                 |
| Osmium                        | Os                                                             | 190.2    | 22.61 <sup>20</sup>              | 3045                       | 5225                     | s molten alkali or oxidizing fluxes                                                  |
| hexafluoride                  | OsF <sub>6</sub>                                               | 304.2    |                                  | 32.1                       | 45.9                     | hyd aq                                                                               |
| tetrachloride                 | OsCl <sub>4</sub>                                              | 332.0    | 4.38 <sup>20</sup>               | subl 450                   |                          | slow hyd aq                                                                          |
| tetraoxide                    | OsO <sub>4</sub>                                               | 254.20   | 4.91                             | 40.6                       | 130.0                    | g/100 mL: 7.24 <sup>25</sup> aq; 375 <sup>25</sup> CCl <sub>4</sub> ; s bz, eth, alc |
| Oxygen                        | O <sub>2</sub>                                                 | 31.9988  | 1.331 g/L <sup>20</sup>          | − 218.4                    | − 182.96                 | mL/100 mL <sup>20</sup> : 3.13 aq, 14.3 alc                                          |
| difluoride                    | OF <sub>2</sub>                                                | 54.00    | 2.26 g/L <sup>20</sup>           | − 223.8                    | − 145.3                  | 6.8 mL/100 mL <sup>0</sup> aq                                                        |
| (di-) difluoride              | O <sub>2</sub> F <sub>2</sub>                                  | 70.00    | 1.45 <sup>bp</sup> (lq)          | − 154                      | d − 100                  |                                                                                      |
| Ozone                         | O <sub>3</sub>                                                 | 48.00    | 1.998 g/L <sup>20</sup>          | − 192.5                    | − 111.9                  | 49.4 mL/100 mL <sup>0</sup> aq                                                       |
| Palladium                     | Pd                                                             | 106.42   | 12.023 <sup>20</sup>             | 1555                       | 3167                     | s hot HNO <sub>3</sub> , H <sub>2</sub> SO <sub>4</sub>                              |
| acetate                       | Pd(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> | 224.49   |                                  | 205 d                      |                          | i aq, alc; s acet, chl, eth                                                          |
| chloride                      | PdCl <sub>2</sub>                                              | 177.30   | 4.0 <sup>18</sup>                | 680                        | d > 680                  | s alc, acet, HCl                                                                     |
| nitrate                       | Pd(NO <sub>3</sub> ) <sub>2</sub>                              | 230.42   |                                  | d                          |                          | s dil HNO <sub>3</sub>                                                               |
| oxide                         | PdO                                                            | 122.40   | 8.70 <sup>20</sup>               | 879 d                      |                          | s 48% HBr; sl s aqua regia                                                           |
| Perchloryl fluoride           | ClO <sub>3</sub> F                                             | 102.46   | 0.637 g/L                        | − 147.74                   | − 46.67                  |                                                                                      |
| Phosphorus (white)            | P <sub>4</sub> molecules                                       | 123.8950 | 1.823 <sup>25</sup>              | 44.15                      | 280.3                    | g/100 mL: 2.86 bz, 2.50 chl, 1.25 CS <sub>2</sub> ; 0.025 abs alc, 1.0 eth           |
| (red)                         | P <sub>4</sub>                                                 | 123.8950 | 2.34                             | 597                        | subl 416                 | i aq; ignites in air, 260                                                            |
| hydride, <i>see</i> Phosphine |                                                                |          |                                  |                            |                          |                                                                                      |
| pentabromide                  | PBr <sub>5</sub>                                               | 430.56   | 3.46 <sup>20</sup>               | 106 d                      |                          | d aq; s CCl <sub>4</sub> , CS <sub>2</sub>                                           |
| pentachloride                 | PCl <sub>5</sub>                                               | 208.27   | 2.119 <sup>20</sup>              | subl 100                   | 166 d                    | hyd aq; s CCl <sub>4</sub> , CS <sub>2</sub>                                         |
| pentafluoride                 | PF <sub>5</sub>                                                | 125.98   | 5.805 g/L                        | − 93.8                     | − 84.6                   | hyd aq                                                                               |
| pentoxide (dimer)             | P <sub>4</sub> O <sub>10</sub>                                 | 283.88   | 2.30                             | 340                        | subl 360                 | d aq; s H <sub>2</sub> SO <sub>4</sub>                                               |
| pentasulfide                  | P <sub>2</sub> S <sub>5</sub>                                  | 222.29   | 2.09                             | 288                        | 514                      | hyd aq; s alkali; 0.222 <sup>17</sup> CS <sub>2</sub>                                |
| tribromide                    | PBr <sub>3</sub>                                               | 270.73   | 2.85 <sup>15</sup>               | − 41.5                     | 173.2                    | d aq, alc; s acet, CS <sub>2</sub>                                                   |
| trichloride                   | PCl <sub>3</sub>                                               | 137.35   | 1.575 <sup>20</sup> <sub>4</sub> | − 93.6                     | 76.1                     | d aq, alc; s bz, chl                                                                 |
| trifluoride                   | PF <sub>3</sub>                                                | 87.98    | 3.907 g/L                        | − 151.30                   | − 101.38                 | hyd aq                                                                               |
| trioxide (dimer)              | P <sub>4</sub> O <sub>6</sub>                                  | 219.90   | 2.136 <sup>20</sup> <sub>4</sub> | 23.8                       | 173 (N <sub>2</sub> atm) | hyd aq; s bz, CS <sub>2</sub>                                                        |
| (tetra-) triselenide          | P <sub>4</sub> Se <sub>3</sub>                                 | 360.80   | 1.31                             | 245–246                    | 360–400                  | flammable in air; s bz, acet, chl, CS <sub>2</sub>                                   |
| (tetra-) trisulfide           | P <sub>4</sub> S <sub>3</sub>                                  | 220.09   | 2.03 <sup>17</sup>               | 167                        | 407                      | 100 g/100 mL <sup>17</sup> CS <sub>2</sub> ; s toluene                               |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| 3.42 | Name                           | Formula                        | Formula weight | Density                   | Melting point,<br>°C      | Boiling point,<br>°C      | Solubility in<br>100 parts solvent                                                      |
|------|--------------------------------|--------------------------------|----------------|---------------------------|---------------------------|---------------------------|-----------------------------------------------------------------------------------------|
|      |                                |                                |                |                           |                           |                           |                                                                                         |
|      | Phosphine                      | PH <sub>3</sub>                | 34.00          | 1.529 g/L                 | − 133.81                  | − 87.78                   | mL/100 mL <sup>17</sup> : 1025 CS <sub>2</sub> , 726 bz,<br>319 HOAc, 26 aq; s alc, eth |
|      | Phosphonium iodide             | PH <sub>4</sub> I              | 161.91         | 2.86                      | 18.5                      | subl 62.5                 | d aq                                                                                    |
|      | Phosphoryl chloride difluoride | POClF <sub>2</sub>             | 120.43         | 1.656 <sup>0</sup>        | − 96.4                    | 3.1                       |                                                                                         |
|      | dichloride fluoride            | POCl <sub>2</sub> F            | 136.89         | 1.5497 <sup>20</sup>      | − 80.1                    | 52.90                     |                                                                                         |
|      | tribromide                     | POBr <sub>3</sub>              | 286.72         | 2.822                     | 56                        | 191.7 d                   | s bz, CS <sub>2</sub> , eth                                                             |
|      | trichloride                    | POCl <sub>3</sub>              | 153.35         | 1.645 <sup>25</sup>       | 1.25                      | 105                       | d aq, alc                                                                               |
|      | Platinum                       | Pt                             | 195.08         | 21.09 <sup>20</sup>       | 1769                      | 3824                      | s aqua regia, fused alkali                                                              |
|      | (II) chloride                  | PtCl <sub>2</sub>              | 266.00         | 5.87                      | d 581                     |                           | i aq, alc; s HCl, NH <sub>4</sub> OH                                                    |
|      | (IV) chloride                  | PtCl <sub>4</sub>              | 336.90         | 4.303 <sup>25</sup>       | d 370                     |                           | 143 g/100 mL <sup>25</sup> aq                                                           |
|      | (VI) fluoride                  | PtF <sub>6</sub>               | 309.08         | 3.826 (lq)                | 61.3                      | 69.14                     |                                                                                         |
|      | (II) oxide                     | PtO                            | 211.09         | 14.9 <sup>15</sup>        | d 550                     |                           | i aq; s HCl                                                                             |
|      | (IV) oxide                     | PtO <sub>2</sub>               | 227.09         | 10.2                      | 450                       |                           | i aqua regia                                                                            |
|      | (IV) sulfide                   | PtS <sub>2</sub>               | 259.22         | 7.66                      | d 225                     |                           | s HCl, HNO <sub>3</sub>                                                                 |
|      | Plutonium                      | Pu                             | 239.052        | 19.816 <sup>20</sup>      | 639.5                     | 3230                      | i aq; s acids                                                                           |
|      | (III) bromide                  | PuBr <sub>3</sub>              | 478.79         | 6.69                      | 681                       | d > 1300                  | s aq                                                                                    |
|      | (III) chloride                 | PuCl <sub>3</sub>              | 345.42         | 5.70                      | 760                       | 1767                      | i aq; v s acids                                                                         |
|      | (III) fluoride                 | PuF <sub>3</sub>               | 296.06         | 9.32                      | 1425                      | d 2000                    | hyd aq                                                                                  |
|      | (IV) fluoride                  | PuF <sub>4</sub>               | 315.05         | 7.00                      | 1037 d                    |                           | i aq                                                                                    |
|      | (VI) fluoride                  | PuF <sub>6</sub>               | 353.05         | 4.86                      | 51.59                     | 62.16                     |                                                                                         |
|      | (II) hydride                   | PuH <sub>2</sub>               | 241.08         | 10.40                     | ca. 727                   |                           |                                                                                         |
|      | (III) hydride                  | PuH <sub>3</sub>               | 242.08         | 9.61                      | ca. 327                   |                           |                                                                                         |
|      | (II) oxide                     | PuO                            | 255.05         | 13.9                      | 1900                      |                           |                                                                                         |
|      | (III) oxide                    | Pu <sub>2</sub> O <sub>3</sub> | 526.12         | 10.2                      | 2085 (in He)              |                           |                                                                                         |
|      | (IV) oxide                     | PuO <sub>2</sub>               | 271.05         | 11.46                     | 2390 (in He)              | d 2800                    |                                                                                         |
|      | (III) sulfide                  | Pu <sub>2</sub> S <sub>3</sub> | 574.30         | 9.95                      | 1727                      |                           |                                                                                         |
|      | Polonium                       | Po                             | 208.9824       | 9.196 alpha<br>9.398 beta | 254                       | 962                       | sl s aq; s acids                                                                        |
|      | (IV) chloride                  | PoCl <sub>4</sub>              | 350.79         |                           | 300 (in Cl <sub>2</sub> ) | 390 (in Cl <sub>2</sub> ) | sl hyd aq; v s HCl; s alc, acet                                                         |
|      | (IV) oxide                     | PoO                            | 240.98         | d 550                     |                           |                           | v s dilute HCl                                                                          |

|                                     |                                                                                |         |                     |                           |                       |                                                 |
|-------------------------------------|--------------------------------------------------------------------------------|---------|---------------------|---------------------------|-----------------------|-------------------------------------------------|
| Potassium                           | K                                                                              | 39.0983 | 0.89                | 63.38                     | 759                   | d aq to KOH; s acids                            |
| acetate                             | KC <sub>2</sub> H <sub>3</sub> O <sub>2</sub>                                  | 98.14   | 1.57                | 292                       |                       | g/100 mL: 200 aq, 34 alc                        |
| arsenate                            | K <sub>3</sub> AsO <sub>4</sub>                                                | 256.21  | 2.8                 | 1310                      |                       | 19 g/100 mL aq; slowly s glyc; s alc            |
| borate(1—)                          | KBO <sub>2</sub>                                                               | 81.91   |                     | 947                       | 1401                  | 71 g/100 mL <sup>30</sup> aq                    |
| bromate                             | KBrO <sub>3</sub>                                                              | 167.00  | 3.27                | ≈350                      | d 370                 | 6.9 g/100 mL <sup>20</sup> aq                   |
| bromide                             | KBr                                                                            | 119.00  | 2.75                | 734                       | 1435                  | g/100 mL: 65 <sup>20</sup> aq, 22 glyc, 0.4 alc |
| carbonate                           | K <sub>2</sub> CO <sub>3</sub>                                                 | 138.21  | 2.29                | 901                       | d to K <sub>2</sub> O | 90 g/100 mL <sup>20</sup> aq; i alc             |
| chlorate                            | KClO <sub>3</sub>                                                              | 122.55  | 2.32                | 368                       | d >400                | g/100 mL: 7.3 <sup>20</sup> aq, 2 glyc          |
| chloride                            | KCl                                                                            | 74.55   | 1.988               | 771                       | 1437                  | g/100 mL: 34 <sup>20</sup> aq, 7 glyc, 0.4 alc  |
| chromate(VI)                        | K <sub>2</sub> CrO <sub>4</sub>                                                | 194.19  | 2.732               | 975                       |                       | 64 g/100 mL <sup>20</sup> aq; i alc             |
| citrate hydrate                     | K <sub>3</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> · H <sub>2</sub> O | 324.42  | 1.98                | anhyd 180                 | d 230                 | g/100 mL: 154 aq; 40 glyc                       |
| cyanate                             | KOCN                                                                           | 81.11   | 2.05                | d ≈700                    |                       | s aq; sl s alc                                  |
| cyanide                             | KCN                                                                            | 65.12   | 1.55                | 634                       | 1625                  | g/100 mL: 50 aq, 50 glyc, 4 MeOH                |
| dichromate(VI)                      | K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>                                  | 294.19  | 2.676 <sup>25</sup> | 398                       | d 500                 | 11.7 g/100 mL <sup>20</sup> aq                  |
| dicyanoargentate(I)                 | K[Ag(CN) <sub>2</sub> ]                                                        | 199.01  | 2.36                |                           |                       | 25 g/100 mL <sup>30</sup> aq                    |
| dihydrogen arsenate                 | KH <sub>2</sub> AsO <sub>4</sub>                                               | 180.03  | 2.867               | 288                       |                       | g/100 mL: 19 <sup>6</sup> aq, 63 glyc; i alc    |
| dihydrogen phosphate                | KH <sub>2</sub> PO <sub>4</sub>                                                | 136.09  | 2.338               | d 400 (KPO <sub>3</sub> ) |                       | 22.6 g/100 mL <sup>20</sup> aq; i alc           |
| dioxide                             | KO <sub>2</sub>                                                                | 71.10   | 2.14                | 509                       | d                     | v s aq with decomposition                       |
| diphosphate(V) 3-water              | K <sub>4</sub> P <sub>2</sub> O <sub>7</sub> · 3H <sub>2</sub> O               | 384.38  | 2.33                | anhyd 300                 | mp: 1090              | s aq; i alc                                     |
| disulfate(IV)                       | K <sub>2</sub> S <sub>2</sub> O <sub>5</sub>                                   | 222.32  |                     |                           |                       | s aq; flammable if ground                       |
| disulfate(VI) (pyrosulfate)         | K <sub>2</sub> S <sub>2</sub> O <sub>7</sub>                                   | 254.32  | 2.28                | ≈325                      |                       | s aq                                            |
| ethyldithiocarbonate                | KOCSSC <sub>2</sub> H <sub>5</sub>                                             | 160.30  | 1.558               | d 200                     |                       | v s aq                                          |
| fluoride                            | KF                                                                             | 58.10   | 2.48                | 859.9                     | 1505                  | 95 g/100 mL <sup>20</sup> aq                    |
| formate                             | KCHO                                                                           | 84.12   | 1.91                | 167.5                     | d >mp                 | 250 g/100 mL aq                                 |
| gluconate                           | KC <sub>6</sub> H <sub>11</sub> O <sub>7</sub>                                 | 234.25  |                     | d 180                     |                       | v s aq; i alc, bz, chl                          |
| heptaiodobis-muthate(III)(4—)       | K <sub>4</sub> [BiI <sub>7</sub> ]                                             | 1253.82 |                     |                           |                       | d aq; s alkali iodide solutions                 |
| hexachloroplatinate(IV)             | K <sub>2</sub> [PtCl <sub>6</sub> ]                                            | 485.99  | 3.50                | d 250                     |                       | 0.48 <sup>20</sup> aq                           |
| hexacyanoferrate(II) 3-water        | K <sub>4</sub> [Fe(CN) <sub>6</sub> ] · 3H <sub>2</sub> O                      | 422.39  | 1.85                | anhyd 100                 | d                     | 28 g/100 mL <sup>20</sup> aq                    |
| hexacyanoferrate(III)               | K <sub>3</sub> [Fe(CN) <sub>6</sub> ]                                          | 329.25  | 1.89                | d                         |                       | 40 g/100 mL <sup>20</sup> aq (slow); sl s alc   |
| hexafluorosilicate                  | K <sub>2</sub> [SiF <sub>6</sub> ]                                             | 220.27  | 2.27                | d                         |                       | sl s aq; i alc                                  |
| hexafluorozirconate                 | K <sub>2</sub> [ZrF <sub>6</sub> ]                                             | 283.41  | 3.58                |                           |                       | 2.7 g/100 mL <sup>20</sup> aq                   |
| hexanitritocobaltate(III) 1.5-water | K <sub>3</sub> [Co(NO <sub>2</sub> ) <sub>6</sub> ] · 1.5H <sub>2</sub> O      | 479.30  |                     | d 200                     |                       | 0.089 <sup>18</sup> aq; s HOAc; v sl s alc      |
| hydride                             | KH                                                                             | 40.11   | 1.43                | 417 d                     |                       | d aq                                            |
| hydrogen carbonate                  | KHCO <sub>3</sub>                                                              | 100.11  | 2.17                | d >100                    |                       | 34 g/100 mL <sup>20</sup> aq; i alc             |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                                     | Formula                                                                                            | Formula weight | Density             | Melting point,<br>°C                              | Boiling point,<br>°C                              | Solubility in<br>100 parts solvent                             |
|------------------------------------------|----------------------------------------------------------------------------------------------------|----------------|---------------------|---------------------------------------------------|---------------------------------------------------|----------------------------------------------------------------|
| Potassium ( <i>continued</i> )           |                                                                                                    |                |                     |                                                   |                                                   |                                                                |
| hydrogen difluoride                      | KHF                                                                                                | 78.10          | 2.37                | 238.80                                            | d 477                                             | 39 g/100 mL <sup>20</sup> aq; s alc                            |
| hydrogen phosphate                       | K <sub>2</sub> HPO <sub>4</sub>                                                                    | 174.18         |                     | d to K <sub>2</sub> P <sub>2</sub> O <sub>7</sub> |                                                   | 150 g/100 mL aq                                                |
| hydrogen phthalate                       | KHC <sub>8</sub> H <sub>4</sub> O <sub>4</sub>                                                     | 204.22         | 1.636               | d                                                 |                                                   | 8.3 g/100 mL aq; sl s alc                                      |
| hydrogen sulfate                         | KHSO <sub>4</sub>                                                                                  | 136.17         | 2.24                | 197                                               | d to K <sub>2</sub> S <sub>2</sub> O <sub>7</sub> | 48 g/100 mL <sup>20</sup> aq                                   |
| hydrogen sulfide                         | KHS                                                                                                | 72.17          | 1.70                | ≈455                                              |                                                   | s aq, alc                                                      |
| hydrogen tartrate                        | KHC <sub>4</sub> H <sub>4</sub> O <sub>6</sub>                                                     | 188.18         | 1.956               |                                                   |                                                   | 0.5 <sup>20</sup> aq; s acids; v sl s alc                      |
| hydroxide                                | KOH                                                                                                | 56.11          | 2.044               | 406                                               | 1323                                              | g/100 mL: 112 <sup>20</sup> aq, 33 alc, 40 glyc                |
| iodate                                   | KIO <sub>3</sub>                                                                                   | 214.00         | 3.89                | 560 d                                             |                                                   | 8.1 g/100 mL <sup>20</sup> aq; i alc                           |
| iodide                                   | KI                                                                                                 | 166.00         | 3.12                | 681                                               | 1345                                              | g/100 mL: 144 <sup>20</sup> aq, 4.5 alc, 50 glyc               |
| manganate(VI)                            | K <sub>2</sub> MnO <sub>4</sub>                                                                    | 197.13         |                     | 190 d                                             |                                                   | s aq; stable in KOH                                            |
| molybdate(VI)                            | K <sub>2</sub> MoO <sub>4</sub>                                                                    | 238.14         | 2.3                 | 919                                               | d 1400                                            | 160 g/100 mL aq                                                |
| nitrate                                  | KNO <sub>3</sub>                                                                                   | 101.10         | 2.11                | 333                                               | d 400                                             | g/100 mL: 32 <sup>20</sup> aq, 0.16 alc, s glyc                |
| nitrite                                  | KNO <sub>2</sub>                                                                                   | 85.10          | 1.915               | 441                                               | d 350                                             | 306 g/100 mL <sup>20</sup> aq; sl s alc                        |
| oxalate hydrate                          | K <sub>2</sub> C <sub>2</sub> O <sub>4</sub> · H <sub>2</sub> O                                    | 184.23         | 2.13                | anhyd 160                                         | d to K <sub>2</sub> CO <sub>3</sub>               | 36 g/100 mL <sup>20</sup> aq                                   |
| oxide                                    | K <sub>2</sub> O                                                                                   | 94.20          | 2.35                | 350 d                                             |                                                   | d aq to KOH, s alc                                             |
| oxobisoxalatodiaquatitanate(IV)          | K <sub>2</sub> [TiO(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ] | 354.18         |                     |                                                   |                                                   | v s aq                                                         |
| perchlorate                              | KClO <sub>4</sub>                                                                                  | 138.55         | 2.52                | d 400                                             |                                                   | 2.04 <sup>25</sup> aq; 0.0036 <sup>25</sup> BuOH; 0.0013 EtOAc |
| periodate                                | KIO <sub>4</sub>                                                                                   | 230.010        | 3.618               | 582                                               |                                                   | 0.42 <sup>20</sup> aq, sl s KOH                                |
| permanganate                             | KMnO <sub>4</sub>                                                                                  | 158.03         | 2.7                 | d 240 → O <sub>2</sub>                            |                                                   | 6.34 g/100 mL <sup>20</sup> aq; d HCl                          |
| peroxide                                 | K <sub>2</sub> O <sub>2</sub>                                                                      | 110.20         |                     | 490                                               |                                                   | d aq                                                           |
| peroxodicarbonate hydrate                | K <sub>2</sub> C <sub>2</sub> O <sub>6</sub> · H <sub>2</sub> O                                    | 216.24         |                     |                                                   |                                                   | 6.5 g/100 mL aq; d hot aq                                      |
| peroxodisulfate                          | K <sub>2</sub> S <sub>2</sub> O <sub>8</sub>                                                       | 270.32         | 2.48                | d 100                                             |                                                   | 2.5 g/100 mL <sup>20</sup> aq; i alc                           |
| perrhenate                               | KReO <sub>4</sub>                                                                                  | 289.30         | 4.38                | 555                                               | 1370                                              | 0.99 <sup>20</sup> aq                                          |
| phenolsulfonate hydrate                  | KC <sub>6</sub> H <sub>4</sub> (OH)SO <sub>3</sub> · H <sub>2</sub> O                              | 240.28         | 1.87                |                                                   |                                                   | s aq, alc                                                      |
| phosphate                                | K <sub>3</sub> PO <sub>4</sub>                                                                     | 212.27         | 2.564 <sup>17</sup> | 1340                                              |                                                   | 50.8 g/100 mL <sup>20</sup> aq; i alc                          |
| selenocyanate                            | KSeCN                                                                                              | 144.08         |                     | d 100                                             |                                                   | s aq                                                           |
| silicate(2-)                             | K <sub>2</sub> SiO <sub>3</sub>                                                                    | 154.29         |                     | 976                                               |                                                   | s aq                                                           |
| sodium hexanitritocobaltate(III) hydrate | K <sub>2</sub> Na[Co(NO <sub>2</sub> ) <sub>6</sub> ] · H <sub>2</sub> O                           | 454.18         | 1.633               | d 135                                             |                                                   | 0.07 aq                                                        |

|                                |                                                                                    |          |                                   |                                        |               |                                                             |
|--------------------------------|------------------------------------------------------------------------------------|----------|-----------------------------------|----------------------------------------|---------------|-------------------------------------------------------------|
| sodium tartrate 4-water        | $\text{KNaC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$                      | 282.23   | 1.790                             | 70–80                                  | anhyd 130–140 | 54 g/100 mL <sup>15</sup> aq                                |
| sorbate                        | $\text{KC}_6\text{H}_7\text{O}_2$                                                  | 150.22   | 1.363 <sub>20</sub> <sup>25</sup> | d > 270                                |               | g/100 mL: 58.2 <sup>20</sup> aq, 6.5 alc                    |
| stannate(IV) 3-water           | $\text{K}_2\text{SnO}_3 \cdot 3\text{H}_2\text{O}$                                 | 298.94   | 3.197                             | anhyd 140                              |               | 100 g/100 mL <sup>20</sup> aq; i alc                        |
| stearate                       | $\text{KOOCC}_{17}\text{H}_{35}$                                                   | 322.57   |                                   |                                        |               | readily soluble hot aq or alc                               |
| sulfate                        | $\text{K}_2\text{SO}_4$                                                            | 174.26   | 2.66                              | 1069                                   | 1670          | g/100 mL: 11 <sup>20</sup> aq, 1.3 glyc, i alc              |
| sulfide                        | $\text{K}_2\text{S}$                                                               | 110.26   | 1.74                              | 948                                    |               |                                                             |
| sulfite 2-water                | $\text{K}_2\text{SO}_3 \cdot 2\text{H}_2\text{O}$                                  | 194.29   |                                   | d                                      |               | 28.6 g/100 mL <sup>20</sup> aq                              |
| tartrate hemihydrate           | $\text{K}_2\text{C}_4\text{H}_4\text{O}_6 \cdot 0.5\text{H}_2\text{O}$             | 235.28   | 1.98                              | anhyd 155                              | d 200         | 138 g/100 mL <sup>20</sup> aq                               |
| tellurate(IV)                  | $\text{K}_2\text{TeO}_3$                                                           | 253.79   |                                   |                                        |               | s aq                                                        |
| tetrachloroaurate(III)         | $\text{K}[\text{AuCl}_4]$                                                          | 377.88   | 3.75                              | d 357                                  |               | 61.8 g/100 mL <sup>20</sup> aq                              |
| tetrafluoroborate              | $\text{K}[\text{BF}_4]$                                                            | 125.90   | 2.505 <sub>4</sub> <sup>20</sup>  | 530                                    |               | 0.45 <sup>20</sup> aq                                       |
| tetrahydridoborate             | $\text{K}[\text{BH}_4]$                                                            | 53.94    | 1.11                              | d 497                                  |               | g/100 mL: 21 <sup>25</sup> aq, 3.5 <sup>20</sup> MeOH       |
| tetraiodocadmiate 2-water      | $\text{K}_4[\text{CdI}_4] \cdot 2\text{H}_2\text{O}$                               | 698.21   | 3.359 <sub>4</sub> <sup>21</sup>  |                                        |               | g/100 mL: 137 <sup>15</sup> aq, 71 <sup>15</sup> alc, 4 eth |
| tetraiodomercurate(II)         | $\text{K}_2[\text{HgI}_4]$                                                         | 786.48   |                                   |                                        |               | v s aq; s alc, acet, eth                                    |
| thiocyanate                    | $\text{KSCN}$                                                                      | 97.18    | 1.89                              | 173                                    | d 500         | g/100 mL: 217 <sup>20</sup> aq, 200 acet, 8 alc             |
| thiosulfate                    | $\text{K}_2\text{S}_2\text{O}_3$                                                   | 190.33   |                                   | d 400                                  |               | 155 g/100 mL <sup>20</sup> aq; i alc                        |
| trihydrogen bisoxalate 2-water | $\text{KH}_3(\text{C}_2\text{O}_4) \cdot 2\text{H}_2\text{O}$                      | 254.20   | 1.836                             | d                                      |               | 1.8 aq                                                      |
| trisoxalatoantimonate(III)     | $\text{K}_3[\text{Sb}(\text{C}_2\text{O}_4)_3]$                                    | 503.12   |                                   |                                        |               | a aq                                                        |
| trithiocarbonate               | $\text{K}_2\text{CS}_3$                                                            | 186.41   |                                   | d                                      |               | v s aq                                                      |
| uranyl(VI) acetate hydrate     | $\text{K}(\text{UO}_2)(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot \text{H}_2\text{O}$ | 504.28   | 3.296 <sup>15</sup>               | anhyd 275                              |               | s aq                                                        |
| Praseodymium                   | Pr                                                                                 | 140.9077 | 6.475 $\alpha$ -form              | 935                                    | 3520          | s hot water and acids                                       |
| chloride                       | $\text{PrCl}_3$                                                                    | 247.27   | 4.0                               | 769 to 782                             | 1710          | 104 g/100 mL <sup>13</sup> aq; s alc                        |
| (III) oxide                    | $\text{Pr}_2\text{O}_3$                                                            | 329.81   | 7.07                              | oxidizes to $\text{Pr}_6\text{O}_{11}$ |               | i aq; s acids                                               |
| (IV)                           | $\text{PrO}_2$                                                                     | 172.91   | 6.82                              | tr 350 to $\text{Pr}_6\text{O}_{11}$   |               |                                                             |
| Promethium-147                 | Pm                                                                                 | 146.915  | 7.22                              | 1080                                   | 3000 est      |                                                             |
| bromide                        | $\text{PmBr}_3$                                                                    | 386.7    | 5.38                              | 727                                    | 1667          | s aq                                                        |
| chloride                       | $\text{PmCl}_3$                                                                    | 153.4    |                                   | 737                                    | 1670          | s aq                                                        |
| Protoactinium                  | Pa                                                                                 | 231.0359 | 15.37                             | 1568(8)                                | 4227          |                                                             |
| (IV) chloride                  | $\text{PaCl}_4$                                                                    | 372.85   | 4.72                              | subl 400                               |               | i aq; s HCl                                                 |
| (V) chloride                   | $\text{PaCl}_5$                                                                    | 408.31   | 3.74                              | 301                                    | 420           | hyd aq; s THF, $\text{CH}_3\text{CN}$                       |
| Radium                         | Ra                                                                                 | 226.03   | 5.5                               | 700.1                                  | 1737          | d aq; s acids                                               |
| bromide                        | $\text{RaBr}_2$                                                                    | 385.88   | 5.79                              | 728                                    | subl 900      | s aq                                                        |
| chloride                       | $\text{RaCl}_2$                                                                    | 296.93   | 4.91                              | 1000                                   |               | s aq                                                        |
| Radon                          | Rn                                                                                 | 222.0    | 9.73 g/L                          | – 71                                   | – 62          | 23 mL/100 mL <sup>20</sup> aq; s org solv                   |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| 3.46 | Name                                          | Formula                                           | Formula weight | Density             | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                     |
|------|-----------------------------------------------|---------------------------------------------------|----------------|---------------------|----------------------|----------------------|--------------------------------------------------------|
|      |                                               |                                                   |                |                     |                      |                      |                                                        |
|      | Rhenium                                       | Re                                                | 186.207        | 21.02               | 3180                 | 5678                 | s HNO <sub>3</sub>                                     |
|      | chloride trioxide                             | ReClO <sub>3</sub>                                | 269.66         |                     | 4.5                  | 128                  | hyd in water to HReO <sub>4</sub> ; s CCl <sub>4</sub> |
|      | (IV) fluoride                                 | ReF <sub>4</sub>                                  | 262.20         | 5.38                | 124.5                | 795                  | hyd aq                                                 |
|      | (VI) fluoride                                 | ReF <sub>6</sub>                                  | 300.20         | 3.58                | 18.5                 | 33.8                 | 52.5 g/100 mL anhyd HF; s HNO <sub>3</sub>             |
|      | (VII) fluoride                                | ReF <sub>7</sub>                                  | 319.20         | 3.65                | 48.3                 | 73.7                 | hyd aq                                                 |
|      | (VI) oxide                                    | ReO <sub>3</sub>                                  | 234.20         | 6.9–7.4             | disprop 400          | 750                  | s HNO <sub>3</sub>                                     |
|      | (VII) oxide                                   | Re <sub>2</sub> O <sub>7</sub>                    | 484.41         | 6.1                 | 300.3                | 360.3                | v s aq, org solv                                       |
|      | (VII) sulfide                                 | Re <sub>2</sub> S <sub>7</sub>                    | 596.88         | 4.866               | d 460                |                      | i aq; s HNO <sub>3</sub>                               |
|      | (VI) tetrachloride oxide                      | ReCl <sub>4</sub> O                               | 344.02         | 3.309               | 29.3                 | 225                  | hyd aq; s CCl <sub>4</sub>                             |
|      | Rhodium                                       | Rh                                                | 102.9055       | 12.41 <sup>20</sup> | 1963                 | 3727                 | s fused KHSO <sub>4</sub>                              |
|      | (III) chloride                                | RhCl <sub>3</sub>                                 | 209.26         | 5.38                | d 450                |                      | i aq; s KOH, KCN                                       |
|      | (III) fluoride                                | RhF <sub>3</sub>                                  | 159.90         | 5.4                 | subl 600             |                      | i acids, alkalis                                       |
|      | (III) oxide                                   | Rh <sub>2</sub> O <sub>3</sub>                    | 253.81         | 8.20                | d 1100               |                      | i aq reg, KOH                                          |
|      | tetracarbonyldi- $\mu$ -chloro-<br>dichloride | Rh <sub>2</sub> (CO) <sub>4</sub> Cl <sub>2</sub> | 388.76         |                     | 124–125              |                      | s org solv except hydrocarbons                         |
|      | Rubidium                                      | Rb                                                | 85.4678        | 1.532               | 39.31                | 691                  | d aq to RbOH                                           |
|      | acetate                                       | RbC <sub>2</sub> H <sub>3</sub> O <sub>2</sub>    | 144.52         |                     | 246                  |                      | 86 g/100 mL <sup>45</sup> aq                           |
|      | bromide                                       | RbBr                                              | 165.37         | 3.35                | 682                  | 1346                 | 108 g/100 mL <sup>20</sup> aq                          |
|      | carbonate                                     | Rb <sub>2</sub> CO <sub>3</sub>                   | 230.95         |                     | 837                  | d 900                | g/100 mL: 450 <sup>20</sup> aq, 0.74 <sub>19</sub> alc |
|      | chlorate                                      | RbClO <sub>3</sub>                                | 168.94         | 3.184               | 342                  |                      | 5.4 g/100 mL <sup>20</sup> aq                          |
|      | chloride                                      | RbCl                                              | 120.92         | 2.76                | 715                  | 1390                 | g/100 mL: 91 <sup>20</sup> aq, 1.1 MeOH                |
|      | dihydrogen phosphate                          | RbH <sub>2</sub> PO <sub>4</sub>                  | 182.47         |                     | 840                  |                      | s aq                                                   |
|      | fluoride                                      | RbF                                               | 104.47         | 3.2                 | 833                  | 1410                 | 131 g/100 mL <sup>18</sup> aq                          |
|      | hexachloroplatinate(IV)                       | Rb <sub>2</sub> [PtCl <sub>6</sub> ]              | 578.75         | 3.94                | d                    |                      | 0.028 <sup>20</sup> aq                                 |
|      | hydroxide                                     | RbOH                                              | 102.47         | 3.20                | 301                  |                      | 180 g/100 mL <sup>18</sup> aq; s alc                   |
|      | iodide                                        | RbI                                               | 212.37         | 3.55                | 642                  | 1304                 | 163 g/100 mL <sup>25</sup> aq; s alc                   |
|      | nitrate                                       | RbNO <sub>3</sub>                                 | 147.47         | 3.11                | 305                  |                      | 19.5 g/100 mL <sup>20</sup> aq                         |
|      | oxide                                         | Rb <sub>2</sub> O                                 | 186.93         | 4.0                 | 400 d                |                      | s aq $\rightarrow$ RbOH                                |
|      | sulfate                                       | Rb <sub>2</sub> SO <sub>4</sub>                   | 267.00         | 3.5                 | 1050                 |                      | 48 g/100 mL <sup>20</sup> aq                           |
|      | Ruthenium                                     | Ru                                                | 101.07         | 12.45 <sup>20</sup> | 2334                 | 4150                 | s fused alkali, oxidizing fluxes                       |
|      | (III) chloride (hexagonal)                    | RuCl <sub>3</sub>                                 | 207.43         | 3.11                | d >500               |                      | i aq; s HCl, alc                                       |
|      | (V) fluoride                                  | RuF <sub>5</sub>                                  | 196.06         | 3.90                | 86.5                 | 227                  | d aq                                                   |
|      | (IV) oxide                                    | RuO <sub>2</sub>                                  | 133.07         | 6.97                | d                    |                      | i aq; s fused alkali                                   |



|                                                           |                                                                     |         |                                  |           |          |                                                                                                                                                |
|-----------------------------------------------------------|---------------------------------------------------------------------|---------|----------------------------------|-----------|----------|------------------------------------------------------------------------------------------------------------------------------------------------|
| Samarium                                                  | Sm                                                                  | 150.36  | 7.52                             | 1074      | 1794     | s acids                                                                                                                                        |
| (II) chloride                                             | SmCl <sub>2</sub>                                                   | 221.27  | 3.687                            | 855       | 2030     | s aq dec; i alc                                                                                                                                |
| (III) chloride                                            | SmCl <sub>3</sub>                                                   | 256.72  | 4.46                             | 682       | d        | 93.4 g/100 mL <sup>20</sup> aq                                                                                                                 |
| (III) fluoride                                            | SmF <sub>3</sub>                                                    | 207.36  | 6.643                            | 1306      | 2427     | i aq; s H <sub>2</sub> SO <sub>4</sub>                                                                                                         |
| (III) oxide                                               | Sm <sub>2</sub> O <sub>3</sub>                                      | 348.72  | 8.347                            | 2335      |          | s acids                                                                                                                                        |
| (III) sulfate 8-water                                     | Sm <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O | 733.03  | 2.93                             | anhyd 450 |          | 2.7 g/100 mL <sup>20</sup> aq                                                                                                                  |
| Scandium                                                  | Sc                                                                  | 44.956  | 2.985 hex                        | 1541      | 2836     | d aq                                                                                                                                           |
| chloride                                                  | ScCl <sub>3</sub>                                                   | 151.31  | 2.39                             | 967       | 967      | v s aq; i alc                                                                                                                                  |
| oxide                                                     | Sc <sub>2</sub> O <sub>3</sub>                                      | 137.91  | 3.864                            | 2485      |          | s hot or conc acids                                                                                                                            |
| sulfate 5-water                                           | Sc <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 5H <sub>2</sub> O | 468.17  | 2.519                            | anhyd 250 | d 550    | 54.6 g/100 mL <sup>25</sup> aq                                                                                                                 |
| Selenium (hexagonal)                                      | Se                                                                  | 78.96   | 4.81 <sub>4</sub> <sup>20</sup>  | 217       | 685      | s eth, KOH, KCN; i aq, alc                                                                                                                     |
| (IV) bromide                                              | SeBr <sub>4</sub>                                                   | 398.58  | 4.029                            | 123       |          | d aq; s HBr, chl, CS <sub>2</sub>                                                                                                              |
| (IV) chloride                                             | SeCl <sub>4</sub>                                                   | 220.77  | 2.6                              | 305       | subl 196 | d aq                                                                                                                                           |
| (di-) dibromide                                           | Se <sub>2</sub> Br <sub>2</sub>                                     | 317.73  | 3.604 <sub>4</sub> <sup>15</sup> |           | 225 d    | d aq; s chl, CS <sub>2</sub>                                                                                                                   |
| dibromide oxide                                           | SeBr <sub>2</sub> O                                                 | 254.77  | 3.38 <sup>20</sup>               | 41.6      | 217 d    | d aq                                                                                                                                           |
| (di-) dichloride                                          | Se <sub>2</sub> Cl <sub>2</sub>                                     | 228.83  | 2.774 <sub>4</sub> <sup>25</sup> | − 85      | 127 dec  | d aq; s bz, chl, CS <sub>2</sub>                                                                                                               |
| dichloride oxide                                          | SeCl <sub>2</sub> O                                                 | 165.867 | 2.44                             | 8.5       | 177.2    | d aq; misc bz, chl, CCl <sub>4</sub> , CS <sub>2</sub>                                                                                         |
| difluoride oxide                                          | SeF <sub>2</sub> O                                                  | 132.96  | 2.8                              | 15        | 125      | d aq                                                                                                                                           |
| (IV) fluoride                                             | SeF <sub>4</sub>                                                    | 154.95  | 2.75                             | − 10      | 106      | reacts aq viol; misc alc, eth; s chl                                                                                                           |
| (VI) fluoride                                             | SeF <sub>6</sub>                                                    | 192.95  | 8.467 g/L                        | − 34.6    |          |                                                                                                                                                |
| (di-) hexasulfide                                         | Se <sub>2</sub> S <sub>6</sub>                                      | 350.32  | 2.44                             | 121.5     |          | s CS <sub>2</sub> ; 1.2 g/100 mL <sup>20</sup> bz                                                                                              |
| (IV) oxide                                                | SeO <sub>2</sub>                                                    | 110.96  | 3.95                             | 340       | subl 315 | w/w %: 38 <sup>14</sup> aq, 10 <sup>12</sup> MeOH, 4.35 acet, 6.7 <sup>14</sup> EtOH, 1.1 <sup>12</sup> HOAc; s H <sub>2</sub> SO <sub>4</sub> |
| (tetra-) tetrasulfide                                     | Se <sub>4</sub> S <sub>4</sub>                                      | 444.10  | 3.20                             | 113 d     |          | i aq; 0.04 g/100 mL <sup>20</sup> bz; s CS <sub>2</sub>                                                                                        |
| Silane                                                    | SiH <sub>4</sub>                                                    | 32.12   | 1.409 g/L                        | − 185     | − 111.9  | d aq slowly; i alc, bz, chl, eth                                                                                                               |
| chloro-                                                   | SiH <sub>3</sub> Cl                                                 | 66.56   | 2.921 g/L                        | − 118     | − 30.4   |                                                                                                                                                |
| dichloro-                                                 | SiH <sub>2</sub> Cl <sub>2</sub>                                    | 101.01  | 4.432 g/L                        | − 122     | 8.3      | d aq                                                                                                                                           |
| iodo-                                                     | SiH <sub>3</sub> I                                                  | 158.01  | 2.035                            | − 57      | 45.5     | d aq                                                                                                                                           |
| trichloro-                                                | SiHCl <sub>3</sub>                                                  | 135.45  | 1.331                            | − 128     | 33       | d aq; s bz, chl                                                                                                                                |
| Silicon                                                   | Si                                                                  | 28.0855 | 2.33                             | 1412      | 3265     | s HF + HNO <sub>3</sub> , fused alkali oxides                                                                                                  |
| carbide (beta)                                            | SiC                                                                 | 40.10   | 3.16                             | 2830      |          | s fused alkali oxides                                                                                                                          |
| dioxide (α quartz)                                        | SiO <sub>2</sub>                                                    | 60.08   | 2.648                            | 573 tr    | 2950     | i aq; s HF                                                                                                                                     |
|                                                           |                                                                     |         |                                  | β quartz  |          |                                                                                                                                                |
| dioxide - tungsten trioxide - water (silicotungstic acid) | SiO <sub>2</sub> · 12WO <sub>3</sub> · 26H <sub>2</sub> O           | 3310.66 |                                  |           |          | v s aq, alc                                                                                                                                    |
| disulfide                                                 | SiS <sub>2</sub>                                                    | 92.22   | 2.04                             | 1090      |          | s d aq, alc; i bz                                                                                                                              |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                         | Formula                                        | Formula weight | Density             | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                                        |
|------------------------------|------------------------------------------------|----------------|---------------------|----------------------|----------------------|-------------------------------------------------------------------------------------------|
| Silicon ( <i>continued</i> ) |                                                |                |                     |                      |                      |                                                                                           |
| tetrabromide                 | SiBr <sub>4</sub>                              | 347.70         | 2.81                | 5.2                  | 154                  | hyd aq viol                                                                               |
| tetrachloride                | SiCl <sub>4</sub>                              | 169.90         | 1.5                 | − 68.8               | 57.6                 | hyd aq; s bz, CCl <sub>4</sub> , eth                                                      |
| tetrafluoride                | SiF <sub>4</sub>                               | 104.08         | 4.567 g/L           | − 90.3               | − 86                 | hyd aq; s HF                                                                              |
| tetraiodide                  | SiI <sub>4</sub>                               | 535.70         | 4.1                 | 120.5                | 287.3                | d aq; 2.2 g/100 mL <sup>27</sup> CS <sub>2</sub>                                          |
| (tri-) tetranitride          | Si <sub>3</sub> N <sub>4</sub>                 | 140.28         | 3.17                | 1878                 |                      | i aq; s HF                                                                                |
| Silver                       | Ag                                             | 107.8682       | 10.49               | 961.78               | 2164                 | s HNO <sub>3</sub>                                                                        |
| acetate                      | AgC <sub>2</sub> H <sub>3</sub> O <sub>2</sub> | 166.91         | 3.259               | d                    |                      | 1.04 <sup>20</sup> aq; s dil HNO <sub>3</sub>                                             |
| antimonide                   | Ag <sub>3</sub> Sb                             | 445.35         |                     | 559                  |                      |                                                                                           |
| azide                        | AgN <sub>3</sub>                               | 149.89         | 4.9                 | exp ~ 252            |                      | i aq; s KCN, HNO <sub>3</sub> (explosive)                                                 |
| bromide                      | AgBr                                           | 187.77         | 6.473               | 432                  | 1500                 | i aq; s KCN                                                                               |
| carbonate                    | Ag <sub>2</sub> CO <sub>3</sub>                | 275.75         | 6.077               | 218                  |                      | 0.003 <sup>20</sup> aq; s KCN, HNO <sub>3</sub> , NH <sub>4</sub> OH                      |
| chlorate                     | AgClO <sub>3</sub>                             | 191.32         | 4.430 <sup>20</sup> | 231                  | d 270                | 10 g/100 mL <sup>15</sup> aq                                                              |
| chloride                     | AgCl                                           | 143.32         | 5.56                | 455                  | 1547                 | i aq; 7.7 g/100 mL NH <sub>4</sub> OH, KCN, Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> |
| chromate(VI)                 | Ag <sub>2</sub> CrO <sub>4</sub>               | 331.73         | 5.625 <sup>25</sup> |                      |                      | 0.002 <sup>20</sup> aq; s HNO <sub>3</sub> , NH <sub>4</sub> OH                           |
| cyanide                      | AgCN                                           | 133.89         | 3.95                | 320 d                |                      | i aq; s KCN                                                                               |
| fluoride                     | AgF                                            | 126.87         | 5.852               | 435                  | ≈ 1150               | 182 g/100 mL <sup>20</sup> aq; s HF, CH <sub>3</sub> CN                                   |
| (II) fluoride                | AgF <sub>2</sub>                               | 145.87         | 4.57                | 690                  | d 700                | hyd viol aq                                                                               |
| iodate                       | AgIO <sub>3</sub>                              | 282.77         | 5.525 <sup>20</sup> | > 200                | d                    | 0.053 <sup>25</sup> aq; 40 g/100 mL 10% NH <sub>4</sub> OH                                |
| iodide (alpha)               | AgI                                            | 234.77         | 5.683 <sup>30</sup> | 558                  | 1505                 | i aq; s KCN, KI, (NH <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub>                          |
| nitrate                      | AgNO <sub>3</sub>                              | 169.87         | 4.352 <sup>19</sup> | 212                  | d 440                | g/100 mL: 216 <sup>20</sup> aq, 3.3 alc, 0.4 acet                                         |
| nitrite                      | AgNO <sub>2</sub>                              | 153.87         | 4.453               | d > 140              |                      | 0.33 <sup>25</sup> aq; d dilute acids                                                     |
| oxalate                      | Ag <sub>2</sub> C <sub>2</sub> O <sub>4</sub>  | 303.76         | 5.03 <sup>4</sup>   | explodes 140         |                      | 0.004 <sup>20</sup> aq; s HNO <sub>3</sub> , NH <sub>4</sub> OH                           |
| oxide                        | Ag <sub>2</sub> O                              | 231.73         | 7.22 <sup>25</sup>  | d 200 (d light)      |                      | 0.002 <sup>25</sup> aq; s dil HNO <sub>3</sub> , NH <sub>4</sub> OH                       |
| (II) oxide                   | AgO                                            | 123.87         | 7.483 <sup>25</sup> | d > 100              |                      | i aq; d alk and acids                                                                     |
| perchlorate                  | AgClO <sub>4</sub>                             | 207.32         | 2.806 <sup>25</sup> | d 486                |                      | 557 g/100 mL <sup>20</sup> aq; s bz, glyc, pyr                                            |
| permanganate                 | AgMnO <sub>4</sub>                             | 226.80         | 4.49                | d by light           |                      | 0.9 aq; d alc                                                                             |

|                            |                                                                       |          |                     |                        |                        |                                                                                                   |
|----------------------------|-----------------------------------------------------------------------|----------|---------------------|------------------------|------------------------|---------------------------------------------------------------------------------------------------|
| phosphate                  | $\text{Ag}_3\text{PO}_4$                                              | 418.62   | 6.37                | 849                    |                        | 0.006 aq; v s dil $\text{HNO}_3$ , KCN, $(\text{NH}_4)_2\text{CO}_3$                              |
| selenate(IV)               | $\text{Ag}_2\text{SeO}_3$                                             | 342.69   | 5.93                | 530                    | d > 530                | sl s aq; s $\text{HNO}_3$                                                                         |
| sulfate                    | $\text{Ag}_2\text{SO}_4$                                              | 311.80   | 5.45                | 660                    | d 1085                 | 0.80 <sup>20</sup> aq (slow); s $\text{HNO}_3$ , $\text{NH}_4\text{OH}$ , $\text{H}_2\text{SO}_4$ |
| sulfide (argentite)        | $\text{Ag}_2\text{S}$                                                 | 247.80   | 7.234 <sup>20</sup> | 845                    | d                      | i aq; s $\text{HNO}_3$ , alk CN's                                                                 |
| Sodium                     | Na                                                                    | 22.98977 | 0.968 <sup>20</sup> | 97.82                  | 881.4                  | d aq to NaOH                                                                                      |
| acetate                    | $\text{NaC}_2\text{H}_3\text{O}_2$                                    | 82.03    | 1.528               | 324                    |                        | 75 g/100 mL <sup>20</sup> aq                                                                      |
| acetate 3-water            | $\text{NaC}_2\text{H}_3\text{O}_2 \cdot 3\text{H}_2\text{O}$          | 136.08   | 1.45                | anhyd 120              | d > 120                | g/100 mL: 125 <sup>20</sup> aq, 5.1 alc                                                           |
| aluminate(1-)              | $\text{NaAlO}_2$                                                      | 81.97    | 4.63                | 1650                   |                        | v s aq; i alc                                                                                     |
| aluminum sulfate 12-water  | $\text{NaAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$               | 458.28   | 1.61                | - 60                   |                        | 110 g/100 mL <sup>15</sup> aq; i alc                                                              |
| amide                      | $\text{NaNH}_2$                                                       | 39.01    | 1.39                | 210                    | subl 400               | d > 500, reacts aq viol                                                                           |
| ammonium phosphate 4-water | $\text{NaNH}_4\text{HPO}_4 \cdot 4\text{H}_2\text{O}$                 | 209.07   | 1.54                | ≈ 80                   | anhyd > 280            | 14.3 g/100 mL aq                                                                                  |
| arsenate(III)(1-)          | $\text{NaAsO}_2$                                                      | 129.91   | 1.87                |                        |                        | v s aq; sl s alc                                                                                  |
| ascorbate                  | $\text{NaC}_6\text{H}_7\text{O}_6$                                    | 198.11   |                     | d 218                  |                        | 62 g/100 mL <sup>20</sup> aq                                                                      |
| azide                      | $\text{NaN}_3$                                                        | 65.01    | 1.846 <sup>20</sup> | d to Na + $\text{N}_2$ |                        | 41 g/100 mL <sup>20</sup> aq; 0.3 alc                                                             |
| benzoate                   | $\text{NaO}_2\text{C}_6\text{H}_5$                                    | 144.11   |                     |                        |                        | g/100 mL: 63 <sup>25</sup> aq; 1.3 alc                                                            |
| bismuthate(V)(1-)          | $\text{NaBiO}_3$                                                      | 279.96   |                     | d                      |                        | i cold aq; dec by hot aq & acids                                                                  |
| bismuthide                 | $\text{Na}_3\text{Bi}$                                                | 277.95   |                     | 766                    |                        | d aq                                                                                              |
| bromate                    | $\text{NaBrO}_3$                                                      | 150.89   | 3.34                | 381 d                  |                        | 40 g/100 mL <sup>20</sup> aq; i alc                                                               |
| bromide                    | NaBr                                                                  | 102.89   | 3.200 <sup>20</sup> | 755                    | 1390                   | g/100 mL: 90 <sup>20</sup> aq, 6 alc; 16 MeOH                                                     |
| carbonate                  | $\text{Na}_2\text{CO}_3$                                              | 105.99   | 2.533 <sup>20</sup> | 858.1                  | d                      | 29 g/100 mL <sup>20</sup> aq; s glyc; i alc                                                       |
| carbonate hydrate          | $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$                     | 124.00   | 2.25                | anhyd 100              |                        | g/100 mL: 33 aq, 14 glyc; i alc                                                                   |
| carbonate 10-water         | $\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$                   | 286.14   | 1.46                | 34 d                   |                        | 50 g/100 mL aq; s glyc                                                                            |
| carbonate - hydrogen       | $\text{Na}_2\text{CO}_3 \cdot \text{NaHCO}_3$                         | 226.02   | 2.112               |                        |                        | 13 g/100 mL <sup>0</sup> aq                                                                       |
| carbonate 2-water (trona)  | $\cdot 2\text{H}_2\text{O}$                                           |          |                     |                        |                        |                                                                                                   |
| chlorate(V)                | $\text{NaClO}_3$                                                      | 106.44   | 2.5                 | 248                    | d > 300 → $\text{O}_2$ | g/100 mL: 96 <sup>20</sup> aq, 0.77 alc, 25 glyc                                                  |
| chloride                   | NaCl                                                                  | 58.44    | 2.17                | 800.8                  | 1465                   | g/100 mL: 36 <sup>20</sup> aq, 10 glyc                                                            |
| chlorite                   | $\text{NaClO}_2$                                                      | 90.44    |                     | d 180-200              |                        | 34 g/100 mL <sup>17</sup> aq                                                                      |
| chromate(VI)               | $\text{Na}_2\text{CrO}_4$                                             | 161.97   | 2.72                | 792                    |                        | 84 g/100 mL <sup>20</sup> aq                                                                      |
| citrate 2-water            | $\text{Na}_3\text{C}_6\text{H}_5\text{O}_7 \cdot 2\text{H}_2\text{O}$ | 294.10   |                     | anhyd 150              |                        | 77 g/100 mL <sup>25</sup> aq; i alc                                                               |
| cyanate                    | NaOCN                                                                 | 65.01    | 1.89                | 550                    |                        | s aq d; 0.22 <sup>0</sup> alc                                                                     |
| cyanide                    | NaCN                                                                  | 49.01    | 1.6                 | 563                    |                        | 58.7 g/100 mL <sup>20</sup> aq                                                                    |
| cyanohydrindoborate        | $\text{Na}[\text{BH}_3\text{CN}]$                                     | 62.84    | 1.12                | > 240 d                |                        | g/100 mL: 212 aq, 37.2 THF; v s NaOH; i bz, eth                                                   |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                                     | Formula                                                                                      | Formula weight | Density                          | Melting point,<br>°C    | Boiling point,<br>°C                               | Solubility in<br>100 parts solvent             |
|------------------------------------------|----------------------------------------------------------------------------------------------|----------------|----------------------------------|-------------------------|----------------------------------------------------|------------------------------------------------|
| <b>Sodium (<i>continued</i>)</b>         |                                                                                              |                |                                  |                         |                                                    |                                                |
| dichromate 2-water                       | $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$                                 | 298.00         | 2.348 <sub>4</sub> <sup>25</sup> | anhyd 100; mp<br>356    | d 400                                              | 73.1 g/100 mL <sup>20</sup> aq                 |
| diethyldithiocarbamate                   | $\text{NaS}_2\text{CN}(\text{C}_2\text{H}_5)_2 \cdot 3\text{H}_2\text{O}$                    | 225.31         |                                  | anhyd 94–96             |                                                    | s aq, alc                                      |
| dihydrogen arsenate(V)                   | $\text{NaH}_2\text{AsO}_4 \cdot \text{H}_2\text{O}$                                          | 181.94         | 2.53                             | anhyd 130               | d 200                                              | s aq                                           |
| hydrate                                  |                                                                                              |                |                                  |                         |                                                    |                                                |
| dihydrogen diphos-<br>phate(V)           | $\text{Na}_2\text{H}_2\text{P}_2\text{O}_7$                                                  | 221.94         | 1.9                              | d 220                   |                                                    | 4.5 g/100 mL <sup>0</sup> aq                   |
| dihydrogen phosphate(V)<br>dihydrate     | $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$                                          | 156.01         | 1.91                             | anhyd 100               | d $\text{NaPO}_3$ , 200                            | 71 g/100 mL <sup>0</sup> aq; i alc             |
| dimethylarsenate 3-water<br>(cacodylate) | $\text{NaO}_2\text{As}(\text{CH}_3)_2$                                                       | 214.03         |                                  | anhyd 120               |                                                    | g/100 mL: 200 aq, 40 alc                       |
| dioxide                                  | $\text{NaO}_2$                                                                               | 54.99          |                                  | 552                     |                                                    |                                                |
| diphosphate(V)                           | $\text{Na}_4\text{P}_2\text{O}_7$                                                            | 265.90         | 2.53                             | 988                     |                                                    | 2.26 <sup>0</sup> aq                           |
| dithionate(V) 2-water                    | $\text{Na}_2\text{S}_2\text{O}_6 \cdot 2\text{H}_2\text{O}$                                  | 242.14         | 2.19                             | anhyd 110               | d 267 to<br>$\text{Na}_2\text{SO}_4 + \text{SO}_2$ | 13.4 g/100 mL <sup>20</sup> aq; i alc          |
| dithionate(III)                          | $\text{Na}_2\text{S}_2\text{O}_4$                                                            | 174.11         |                                  | d                       |                                                    | 22 g/100 mL <sup>20</sup> aq; sl s alc         |
| diuranate(VI)                            | $\text{Na}_2\text{U}_2\text{O}_7$                                                            | 634.03         |                                  |                         |                                                    | i aq; s acids                                  |
| dodecylbenzenesulfonate                  | $\text{NaO}_3\text{SC}_6\text{H}_4\text{C}_{12}\text{H}_{25}$                                | 348.49         |                                  |                         |                                                    |                                                |
| dodecylsulfate                           | $\text{NaO}_3\text{SOC}_{12}\text{H}_{25}$                                                   | 288.38         |                                  |                         |                                                    | 10 g/100 mL aq                                 |
| ethoxide                                 | $\text{NaOC}_2\text{H}_5$                                                                    | 68.06          |                                  | >300                    |                                                    | d aq; s abs alc                                |
| ethylenebis(imino-<br>diacetate) (EDTA)  | $(\text{NaOOCCH}_2)_2\text{NC}_2\text{H}_4\text{-}$<br>$\text{N}(\text{CH}_2\text{COONa})_2$ | 380.20         |                                  |                         |                                                    | 103 g/100 mL aq                                |
| ethylsulfate                             | $\text{NaO}_3\text{SOC}_2\text{H}_5$                                                         | 148.12         |                                  |                         |                                                    | 140 g/100 mL aq; s alc                         |
| fluoride                                 | $\text{NaF}$                                                                                 | 41.99          | 2.78                             | 996                     | 1704                                               | 4 g/100 mL <sup>15</sup> aq; i alc             |
| formate                                  | $\text{NaHCO}_2$                                                                             | 68.01          | 1.92                             | 253                     | d >253                                             | 81 g/100 mL <sup>20</sup> aq; s glyc; sl s alc |
| gluconate                                | $\text{NaC}_6\text{H}_{11}\text{O}_7$                                                        | 218.14         |                                  |                         |                                                    | 59 g/100 mL <sup>25</sup> aq; sl s alc; i eth  |
| glycerophosphate                         | $\text{Na}_2\text{C}_3\text{H}_5(\text{OH})_2\text{PO}_4$                                    | 216.04         |                                  | d >130                  |                                                    | 67 g/100 mL aq; i alc                          |
| hexachloroplatinate(IV)<br>6-water       | $\text{Na}_2[\text{PtCl}_6] \cdot 6\text{H}_2\text{O}$                                       | 561.88         | 2.50                             | –6H <sub>2</sub> O, 110 |                                                    | v s aq; s alc                                  |

|                                                                  |                                                                          |        |       |                             |                                |                                                                |
|------------------------------------------------------------------|--------------------------------------------------------------------------|--------|-------|-----------------------------|--------------------------------|----------------------------------------------------------------|
| hexacyanoferrate(II)<br>10-water                                 | $\text{Na}_4[\text{Fe}(\text{CN})_6] \cdot 10\text{H}_2\text{O}$         | 484.06 | 1.46  | anhyd 82                    | d 435                          | 28 g/100 mL <sup>20</sup> aq                                   |
| hexacyanoferrate(III) hy-<br>drate                               | $\text{Na}_3[\text{Fe}(\text{CN})_6] \cdot \text{H}_2\text{O}$           | 298.93 |       |                             |                                | 18.9 g/100 mL <sup>0</sup> aq                                  |
| hexafluoroaluminate                                              | $\text{Na}_3[\text{AlF}_6]$                                              | 209.94 | 2.97  | 1009                        |                                | s aq                                                           |
| hexanitritocobaltate(III)                                        | $\text{Na}_3[\text{Co}(\text{NO}_2)_6]$                                  | 403.98 |       |                             |                                | v s aq; sl s alc                                               |
| hydride                                                          | NaH                                                                      | 24.00  | 1.39  | 425 d                       |                                | ign spontaneously moisture; d alc<br>viol                      |
| hydrogen arsenate(V)<br>7-water                                  | $\text{Na}_2\text{HAsO}_4 \cdot 7\text{H}_2\text{O}$                     | 312.01 | 1.87  | anhyd 130                   | d 150                          | 61 g/100 mL <sup>15</sup> aq; s glyc; sl s alc                 |
| hydrogen carbonate                                               | $\text{NaHCO}_3$                                                         | 84.01  | 2.20  | to $\text{Na}_2\text{CO}_3$ | 270                            | 8 g/100 mL <sup>20</sup> aq; i alc                             |
| hydrogen difluoride                                              | $\text{NaHF}_2$                                                          | 62.00  | 2.08  | d > 160                     |                                | 3.7 g/100 mL <sup>20</sup> aq                                  |
| hydrogen phosphate<br>7-water                                    | $\text{Na}_2\text{HPO}_4 \cdot 7\text{H}_2\text{O}$                      | 268.07 | 1.7   | d                           |                                | 25 g/100 mL <sup>40</sup> aq; v sl s alc                       |
| hydrogen sulfate                                                 | $\text{NaHSO}_4$                                                         | 120.06 | 2.435 | 315                         | d                              | 50 g/100 mL <sup>20</sup> aq; d alc                            |
| hydrogen sulfide                                                 | NaHS                                                                     | 56.06  | 1.79  | 350                         |                                | s aq, alc, eth                                                 |
| hydrogen sulfite                                                 | $\text{NaHSO}_3$                                                         | 104.06 | 1.48  | d                           |                                | g/100 mL: 29 aq, 1.4 alc                                       |
| hydroxide                                                        | NaOH                                                                     | 40.00  | 2.130 | 323                         | 1388                           | g/100 mL: 108 <sup>20</sup> aq, 14 abs alc, 24<br>MeOH; s glyc |
| hydroxymethanesulfinate<br>dihydrate                             | $\text{Na}[\text{HOCH}_2\text{SO}_2] \cdot 2\text{H}_2\text{O}$          | 154.12 |       | 63–64                       | d > 64                         | v s aq; i abs alc, bz, eth                                     |
| hypochlorite 5-water                                             | $\text{NaClO} \cdot 5\text{H}_2\text{O}$                                 | 164.52 | 1.6   | 18                          | d by $\text{CO}_2$ from<br>air | 29 g/100 mL <sup>0</sup> aq                                    |
| iodate                                                           | $\text{NaIO}_3$                                                          | 197.89 | 4.28  | d                           |                                | 8.1 g/100 mL <sup>20</sup> aq                                  |
| iodide                                                           | NaI                                                                      | 149.89 | 3.67  | 660                         | 1304                           | g/100 mL: 200 <sup>20</sup> aq, 100 glyc, 50<br>alc; s acet    |
| lactate                                                          | $\text{NaOOCCHOHCH}_3$                                                   | 112.06 |       | d                           |                                | misc aq, alc                                                   |
| methoxide                                                        | $\text{NaOCH}_3$                                                         | 54.02  |       | > 300                       |                                | d aq; s alc                                                    |
| molybdate(VI) 2-water                                            | $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$                      | 241.95 | ≈ 3.5 | anhyd 100                   | mp 687                         | 65 g/100 mL <sup>20</sup> aq                                   |
| nitrate                                                          | $\text{NaNO}_3$                                                          | 85.00  | 2.26  | 307                         | d ≈ 500                        | g/100 mL: 88 <sup>20</sup> aq, 0.8 alc                         |
| nitrite                                                          | $\text{NaNO}_2$                                                          | 69.00  | 2.17  | 271                         | d > 320                        | 67 g/100 mL <sup>20</sup> aq                                   |
| oxalate                                                          | $\text{Na}_2\text{C}_2\text{O}_4$                                        | 134.00 | 2.34  | d ≈ 250                     |                                | 3.4 g/100 mL <sup>20</sup> aq; i alc                           |
| oxide                                                            | $\text{Na}_2\text{O}$                                                    | 61.98  | 2.27  | dull red heat               | d > 400                        | d aq to NaOH violently                                         |
| pentacyanonitrosylfer-<br>rate(III) 2-water (nitro-<br>prusside) | $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}] \cdot 2\text{H}_2\text{O}$ | 297.65 | 1.72  |                             |                                | 40 g/100 mL <sup>16</sup> aq                                   |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                              | Formula                                                                          | Formula weight | Density | Melting point,<br>°C | Boiling point,<br>°C      | Solubility in<br>100 parts solvent                     |
|-----------------------------------|----------------------------------------------------------------------------------|----------------|---------|----------------------|---------------------------|--------------------------------------------------------|
| Sodium ( <i>continued</i> )       |                                                                                  |                |         |                      |                           |                                                        |
| perchlorate                       | NaClO <sub>4</sub>                                                               | 122.44         | 2.52    | 480 d                |                           | g/100 mL <sup>25</sup> ; 114 aq, 1.5 BuOH, 8.4 EtOAc   |
| periodate                         | KIO <sub>4</sub>                                                                 | 213.89         | 3.865   | d ≈ 300              |                           | 10.3 g/100 mL <sup>20</sup> aq                         |
| peroxide                          | Na <sub>2</sub> O <sub>2</sub>                                                   | 77.98          | 2.805   | 675                  | d                         | v s aq (dec)                                           |
| peroxoborate 4-water              | NaBO <sub>3</sub> · 4H <sub>2</sub> O                                            | 153.88         |         | d > 60               |                           | 2.5 g/100 mL aq                                        |
| peroxodisulfate(VI)               | Na <sub>2</sub> S <sub>2</sub> O <sub>8</sub>                                    | 238.11         |         | d                    |                           | 55 g/100 mL aq; d by alc                               |
| perrhenate                        | NaReO <sub>4</sub>                                                               | 273.19         | 5.24    | 300                  |                           | 33 g/100 mL <sup>20</sup> aq                           |
| phosphate                         | Na <sub>3</sub> PO <sub>4</sub>                                                  | 163.94         | 2.537   | 1340                 |                           | 12.1 g/100 mL <sup>20</sup> aq                         |
| phosphate 12-water                | Na <sub>3</sub> PO <sub>4</sub> · 12H <sub>2</sub> O                             | 380.12         | 1.62    | 73.4                 | – 11H <sub>2</sub> O, 100 | 28.3 g/100 mL <sup>20</sup> aq; i alc                  |
| phosphinate hydrate               | NaPH <sub>2</sub> O <sub>2</sub> · H <sub>2</sub> O                              | 105.99         |         | anhyd 200            | d to PH <sub>3</sub>      | 100 g/100 mL <sup>20</sup> aq; s glyc, alc             |
| propanoate                        | NaOCC <sub>2</sub> H <sub>5</sub>                                                | 96.06          |         |                      |                           | g/100 mL <sup>25</sup> ; 100 aq, 4.1 alc               |
| salicylate                        | NaOCC <sub>6</sub> H <sub>4</sub> OH                                             | 160.10         |         |                      |                           | g/100 mL: 110 <sup>20</sup> aq, 11 alc, 25 glyc        |
| selenate(VI)                      | Na <sub>2</sub> SeO <sub>4</sub>                                                 | 188.94         | 3.098   |                      |                           | 27 g/100 mL <sup>20</sup> aq                           |
| silicate(2–) meta-                | Na <sub>2</sub> SiO <sub>3</sub>                                                 | 122.06         | 2.614   | 1089                 |                           | s aq; hyd by hot aq; i alc                             |
| silicate(2–) 5-water              | Na <sub>2</sub> SiO <sub>3</sub> · 5H <sub>2</sub> O                             | 212.14         | 1.749   | 72.2                 | anhyd 100                 | v s aq                                                 |
| silicate(4–)                      | Na <sub>4</sub> SiO <sub>4</sub>                                                 | 184.04         |         | 1018                 |                           | s aq                                                   |
| stannate(IV) 3-water              | Na <sub>2</sub> SnO <sub>3</sub> · 3H <sub>2</sub> O                             | 266.71         |         | d 140 (slow)         |                           | 59 g/100 mL <sup>20</sup> aq; i alc                    |
| stearate                          | NaOCC <sub>17</sub> H <sub>35</sub>                                              | 306.47         |         | d                    |                           | sl s aq                                                |
| sulfate                           | Na <sub>2</sub> SO <sub>4</sub>                                                  | 142.04         | 2.7     | 8800                 | d 2227                    | 28 g/100 mL <sup>20</sup> aq                           |
| sulfate 10-water                  | Na <sub>2</sub> SO <sub>4</sub> · 10H <sub>2</sub> O                             | 322.20         | 1.46    | 32.4                 | anhyd 100                 | 67 g/100 mL <sup>25</sup> aq; s glyc; i alc            |
| sulfide                           | Na <sub>2</sub> S                                                                | 78.05          | 1.856   | 1172 vacuo           |                           | 18.6 g/100 mL <sup>20</sup> aq; sl s alc               |
| sulfide 9-water                   | Na <sub>2</sub> S · 9H <sub>2</sub> O                                            | 240.18         | 1.43    | d ≈ 50               |                           | 200 g/100 mL aq; sl s alc                              |
| sulfite                           | Na <sub>2</sub> SO <sub>3</sub>                                                  | 126.04         | 2.63    | d                    |                           | 31 g/100 mL <sup>20</sup> aq; s glyc; i alc            |
| tartrate dihydrate                | Na <sub>2</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 2H <sub>2</sub> O | 230.08         | 1.82    | anhyd ~ 120          |                           | 29 g/100 mL <sup>6</sup> aq; i alc                     |
| tetraborate                       | Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                                    | 201.22         | 2.4     | 742.5                |                           | 2.6 <sup>20</sup> aq                                   |
| tetraborate 10-water (bo-<br>rax) | Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> · 10H <sub>2</sub> O               | 381.37         | 1.73    | 75 d                 | anhyd 320                 | g/100 mL: 6.3 aq, 100 glyc                             |
| tetrachloroaluminate              | Na[AlCl <sub>4</sub> ]                                                           | 191.78         | 2.01    | 151                  |                           | s aq                                                   |
| tetrachloroaurate                 | Na[AuCl <sub>4</sub> ] · 2H <sub>2</sub> O                                       | 397.80         |         | d > 100              |                           | 166 g/100 mL <sup>27</sup> aq; s alc, chl              |
| tetrafluoroborate                 | Na[BF <sub>4</sub> ]                                                             | 109.82         | 2.47    | 384                  | d                         | 108 g/100 mL <sup>27</sup> aq                          |
| tetrahydridoborate                | Na[BH <sub>4</sub> ]                                                             | 37.83          | 1.074   | 497                  | d 315                     | 18 <sup>25</sup> DMF; 16.4 <sup>20</sup> MeOH (reacts) |

|                                        |                                                                   |        |                      |                                    |                         |                                                                 |
|----------------------------------------|-------------------------------------------------------------------|--------|----------------------|------------------------------------|-------------------------|-----------------------------------------------------------------|
| thiocyanate                            | NaSCN                                                             | 81.07  |                      | 287                                |                         | 134 g/100 mL <sup>20</sup> aq                                   |
| thiosulfate                            | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub>                     | 158.11 | 2.345                |                                    |                         | s aq; i alc                                                     |
| thiosulfate 5-water                    | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> · 5H <sub>2</sub> O | 248.19 | 1.69                 | anhyd 100                          | d > 100                 | 70 g/100 mL <sup>20</sup> aq (dec slowly)                       |
| trimetaphosphate 6-water               | (NaPO <sub>3</sub> ) <sub>3</sub> · 6H <sub>2</sub> O             | 414.04 | 1.786                | 53                                 | anhyd 100               | 22 g/100 mL aq; i alc                                           |
| tungstate(VI) dihydrate                | Na <sub>2</sub> WO <sub>4</sub> · 2H <sub>2</sub> O               | 329.85 | 3.25                 | anhyd 100                          | mp: 695.6               | 88 g/100 mL <sup>0</sup> aq; i alc                              |
| vanadate(V)                            | NaVO <sub>3</sub>                                                 | 121.93 |                      |                                    |                         | s hot aq                                                        |
| Srontium                               | Sr                                                                | 87.62  | 2.64                 | 757                                | 1366                    | d to Sr(OH) <sub>2</sub> in water                               |
| bromide                                | SrBr <sub>2</sub>                                                 | 247.43 | 4.216                | 657                                | 2045                    | 100 g/100 mL <sup>20</sup> aq                                   |
| carbonate                              | SrCO <sub>3</sub>                                                 | 147.63 | 3.5                  | d 1100 to SrO<br>+ CO <sub>2</sub> |                         | i aq; s acids                                                   |
| chlorate                               | Sr(ClO <sub>3</sub> ) <sub>2</sub>                                | 254.52 | 3.152                | 120 d → O <sub>2</sub>             |                         | 167 g/100 mL <sup>20</sup> aq                                   |
| chloride                               | SrCl <sub>2</sub>                                                 | 158.53 | 3.052                | 874                                | 1250                    | 52.9 g/100 mL <sup>20</sup> aq                                  |
| chromate(VI)                           | SrCrO <sub>4</sub>                                                | 203.61 | 3.89                 | d                                  |                         | 0.12 <sup>20</sup> aq; s HCl                                    |
| fluoride                               | SrF <sub>2</sub>                                                  | 125.62 | 4.24                 | 1477                               | 2460                    | 0.011 <sup>20</sup> aq; s hot HCl                               |
| hydrogen phosphate                     | SrHPO <sub>4</sub>                                                | 183.60 | 3.544                |                                    |                         | i aq; s acids                                                   |
| hydroxide                              | Sr(OH) <sub>2</sub>                                               | 121.64 | 3.625                | 535                                | — H <sub>2</sub> O, 744 | 0.8 <sup>20</sup> aq                                            |
| iodate                                 | Sr(IO <sub>3</sub> ) <sub>2</sub>                                 | 437.43 | 5.045 <sup>15</sup>  |                                    |                         | 0.03 <sup>15</sup> aq                                           |
| iodide                                 | SrI <sub>2</sub>                                                  | 341.43 | 4.42                 | 402                                | 1773 d                  | 178 g/100 mL <sup>20</sup> aq; s alc                            |
| lactate 3-water                        | Sr(OOCCHOHCH <sub>3</sub> ) <sub>2</sub> · 3H <sub>2</sub> O      | 319.81 |                      | anhyd 150                          |                         | 33 g/100 mL aq                                                  |
| nitrate                                | Sr(NO <sub>3</sub> ) <sub>2</sub>                                 | 211.63 | 2.99                 | 570                                | 645                     | 69.5 g/100 mL <sup>20</sup> aq; sl s alc, acet                  |
| oxide                                  | SrO                                                               | 103.62 | 4.7                  | 2430                               |                         | 0.69 <sup>20</sup> aq                                           |
| perchlorate                            | Sr(ClO <sub>4</sub> ) <sub>2</sub>                                | 286.52 | 3.00 <sup>25</sup>   |                                    |                         | g/100 mL <sup>25</sup> ; 157 aq, 71 BuOH, 77 EtOAc, 90 acet     |
| peroxide                               | SrO <sub>2</sub>                                                  | 119.62 | 4.78                 | 215 d                              |                         | 0.018 <sup>20</sup> aq; d hot aq                                |
| sulfate                                | SrSO <sub>4</sub>                                                 | 183.68 | 3.96                 | 1607                               |                         | 0.013 <sup>20</sup> aq; sl s acid                               |
| sulfide                                | SrS                                                               | 119.69 | 3.70                 | 2227                               |                         | sl s aq; s acid (dec)                                           |
| Sulfinyl bromide (Thionyl)             | SOBr <sub>2</sub>                                                 | 207.87 | 2.688 <sup>20</sup>  | — 52                               | 140                     | hyd aq (slow); misc bz, chl, CCl <sub>4</sub>                   |
| chloride                               | SOCl <sub>2</sub>                                                 | 118.97 | 1.638                | — 104.5                            | 76                      | hyd aq; misc bz, chl, CCl <sub>4</sub>                          |
| fluoride                               | SOF <sub>2</sub>                                                  | 86.06  | 3.776 g/L            | — 129.5                            | — 43.8                  | hyd aq; s bz, chl, eth                                          |
| Sulfonyl chloride (Sulfuryl)           | SO <sub>2</sub> Cl <sub>2</sub>                                   | 134.97 | 1.6674 <sup>20</sup> | — 54.1                             | 69.3                    | hyd aq; misc bz, eth, HOAc                                      |
| diamide                                | SO <sub>2</sub> (NH <sub>2</sub> ) <sub>2</sub>                   | 96.11  | 1.807                | 93                                 | d 250                   | s aq, hot EtOH, acet                                            |
| fluoride                               | SO <sub>2</sub> F <sub>2</sub>                                    | 102.06 | 4.478 g/L            | — 135.8                            | — 55.38                 | mL gas/100 mL: 4 aq, 24 alc, 136 CCl <sub>4</sub> , 210 toluene |
| Sulfur (gamma)                         | S                                                                 | 32.066 | 1.92                 | 106.8                              | 444.72                  | 23 g/100 mL <sup>0</sup> CS <sub>2</sub> ; s alc, bz            |
| (alpha) orthorhombic                   | S <sub>8</sub>                                                    | 256.53 | 2.08 <sup>20</sup>   | tr 94.5 to beta form               | 444.6                   | i aq; s organic solvents                                        |
| (beta) monoclinic tr slowly to rhombic | S <sub>8</sub>                                                    | 256.53 | 1.96                 | 115.21                             | 444.6                   | 23 g/100 mL <sup>0</sup> CS ; s alc, bz                         |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                          | Formula                        | Formula weight | Density            | Melting point,<br>°C | Boiling point,<br>°C | Solubility in<br>100 parts solvent                               |
|-------------------------------|--------------------------------|----------------|--------------------|----------------------|----------------------|------------------------------------------------------------------|
| Sulfur ( <i>continued</i> )   |                                |                |                    |                      |                      |                                                                  |
| (di-) decafluoride            | S <sub>2</sub> F <sub>10</sub> | 254.11         | 2.08               | − 52.7               | 30                   | d fusion with KOH                                                |
| (di-) dichloride              | ClSSCl                         | 135.04         | 1.688              | − 77                 | 137                  | hyd aq; s alc, bz, eth, CS <sub>2</sub> , CCl <sub>4</sub>       |
| dichloride                    | SCl <sub>2</sub>               | 102.97         | 1.622              | − 122                | 59.5                 | hyd aq                                                           |
| dioxide                       | SO <sub>2</sub>                | 64.07          | 2.811 g/L          | − 75.47              | − 10                 | mL/100 mL: 3937 <sup>20</sup> aq, 25 alc, 32 MeOH; s chl, eth    |
| hexafluoride                  | SF <sub>6</sub>                | 146.06         | 6.409 g/L          | − 50.8               | subl − 63.8          | sl s aq; s alc, KOH                                              |
| tetrafluoride                 | SF <sub>4</sub>                | 108.06         | 4.742 g/L          | − 121.0              | − 38                 | d aq viol; v s bz                                                |
| trioxide (alpha)              | SO <sub>3</sub>                | 80.06          |                    | 62.3                 | vp 73mm at 25        | stable modification                                              |
| (beta)                        | SO <sub>3</sub>                | 80.06          |                    | 32.5                 | vp 344mm at 25       |                                                                  |
| (gamma)                       | SO <sub>3</sub>                | 80.06          | 1.92               | 16.8                 | 44.8                 | v s aq (slow)                                                    |
| Sulfuryl, <i>see</i> Sulfonyl |                                |                |                    |                      |                      |                                                                  |
| Tantalum                      | Ta                             | 180.9479       | 16.69              | 2996                 | 5429                 | s HF, fused alkali (slowly)                                      |
| (V) bromide                   | TaBr <sub>5</sub>              | 580.47         | 4.99               | 265                  | 349                  | hyd aq; s abs alc, eth                                           |
| carbide                       | TaC                            | 192.96         | 14.3               | 3880                 | 4780                 | sl s HF                                                          |
| (di-) carbide                 | Ta <sub>2</sub> C              | 373.91         | 15.1               | 3327                 |                      |                                                                  |
| (V) chloride                  | TaCl <sub>5</sub>              | 358.21         | 3.68               | 216                  | 239.3                | hyd aq; s abs alc                                                |
| diboride                      | TaB <sub>2</sub>               | 202.57         | 11.2               | 3140                 |                      |                                                                  |
| (V) fluoride                  | TaF <sub>5</sub>               | 275.94         | 4.74 <sup>20</sup> | 96.8                 | 229.5                | s aq, eth, conc HNO <sub>3</sub>                                 |
| (V) iodide                    | TaI                            | 815.47         | 5.80               | 496                  | 543                  | hyd aq; s eth                                                    |
| nitride                       | TaN                            | 194.95         | 13.7               | 3090                 |                      | sl s aq reg; reacts alkalis                                      |
| (V) oxide                     | Ta <sub>2</sub> O <sub>5</sub> | 441.89         | 8.2                | 1785                 |                      | s HF; d fused KHSO <sub>4</sub> or KOH                           |
| Technetium-98                 | Tc                             | 97.9072        | 11                 | 2157                 | 4265                 | s HNO <sub>3</sub> , aq reg, conc H <sub>2</sub> SO <sub>4</sub> |
| (VI) fluoride                 | TcF <sub>6</sub>               | 212.91         | 3.0                | 37.4                 | 55.3                 | s HCl                                                            |
| (IV) oxide                    | TcO <sub>2</sub>               | 130.91         | 6.9                | subl 1000            |                      | s acid, alkali                                                   |
| (VII) oxide                   | Tc <sub>2</sub> O <sub>7</sub> | 309.81         |                    | 119.5                | 310.6                | s aq                                                             |
| Tellurium                     | Te                             | 127.60         | 6.24               | 449.8                | 989.9                | s HNO <sub>3</sub> , KOH, conc H <sub>2</sub> SO <sub>4</sub>    |
| (IV) bromide                  | TeBr                           | 447.22         | 4.3                | 380                  | ≈ 20 d               | s HBr, eth, HOAc                                                 |
| (II) chloride                 | TeCl <sub>2</sub>              | 198.51         | 6.9                | 208                  | 328                  | disprop with eth, diox; s acid                                   |
| (IV) chloride                 | TeCl <sub>4</sub>              | 269.41         | 3.0                | 225                  | 380                  | hyd aq; s HCl, abs alc, bz                                       |
| (IV) fluoride                 | TeF <sub>4</sub>               | 203.59         |                    | 129                  | d > 195              | d aq                                                             |
| (VI) fluoride                 | TeF <sub>6</sub>               | 241.59         | 10.601 g/L         | − 37.68              | subl − 38.9          | hyd aq, KOH                                                      |



|                              |                                                       |          |                     |                         |                        |                                                |
|------------------------------|-------------------------------------------------------|----------|---------------------|-------------------------|------------------------|------------------------------------------------|
| (IV) iodide                  | TeI <sub>4</sub>                                      | 635.22   | 5.05                | 280                     |                        | hyd aq; s HI, alkali; sl s acet                |
| (IV) oxide                   | TeO <sub>2</sub>                                      | 159.60   | 5.9                 | 733                     | 1245                   | s HCl, HF, NaOH                                |
| Terbium                      | Tb                                                    | 158.9254 | 8.23                | 1356                    | 3230                   | s acids                                        |
| chloride                     | TbCl <sub>3</sub>                                     | 265.28   | 4.35                | 588                     | 1550                   | v s aq                                         |
| nitrate 6-water              | Tb(NO <sub>3</sub> ) <sub>3</sub> · 6H <sub>2</sub> O | 453.03   |                     | 89.3                    |                        | s aq                                           |
| Thallium                     | Tl                                                    | 204.383  | 11.85               | 303.5                   | 1457                   | i aq; s HNO <sub>3</sub>                       |
| (I) bromide                  | TlBr                                                  | 284.29   | 7.5                 | 460                     | 820                    | 0.05 <sup>20</sup> aq; s alc                   |
| (I) carbonate                | Tl <sub>2</sub> CO <sub>3</sub>                       | 468.78   | 7.11                | 272                     |                        | 4.1 g/100 mL <sup>20</sup> aq; i alc           |
| (I) chloride                 | TlCl                                                  | 239.84   | 7.00                | 430                     | 720                    | 0.33 <sup>20</sup> aq; i alc                   |
| (I) cyanide                  | TlCN                                                  | 230.40   | 6.523               | d                       |                        | 16.8 g/100 mL <sup>28</sup> aq; s alc, acid    |
| (I) ethoxide                 | TlOC <sub>2</sub> H <sub>5</sub>                      | 249.44   | 3.49                | — 3                     | d 130                  | s eth; sl s alc; d aq                          |
| (I) fluoride                 | TlF                                                   | 223.38   | 8.36                | 326                     | 826                    | 78.6% <sup>15</sup> aq                         |
| (III) fluoride               | TlF <sub>3</sub>                                      | 261.38   | 8.65                | 550 d                   |                        | d aq                                           |
| (I) iodide (rhombic)         | TlI                                                   | 331.29   | 7.1                 | 442                     | 823                    | i aq, alc; s KI                                |
| (I) nitrate                  | TlNO <sub>3</sub>                                     | 266.39   | 5.55                | 206                     | d 450                  | 9.55 g/100 mL <sup>20</sup> aq; i alc          |
| (I) oxide                    | Tl <sub>2</sub> O                                     | 424.77   | 9.52                | 579                     | 1080                   | v s aq; s acid, alc                            |
| (III) oxide (hexagonal)      | Tl <sub>2</sub> O <sub>3</sub>                        | 456.77   | 10.2                | 834                     | — O <sub>2</sub> , 875 | i aq; d by HCl, H <sub>2</sub> SO <sub>4</sub> |
| (I) selenate(VI)             | Tl <sub>2</sub> SeO <sub>4</sub>                      | 551.73   | 6.875               | >400                    |                        | 2.8 g/100 mL <sup>20</sup> aq; i alc, eth      |
| (I) selenide                 | Tl <sub>2</sub> Se                                    | 487.73   | 9.05                | 340                     |                        | i aq, acid                                     |
| (I) sulfate                  | Tl <sub>2</sub> SO <sub>4</sub>                       | 504.83   | 6.77                | 632                     | d                      | 4.87 g/100 mL <sup>20</sup> aq                 |
| (I) sulfide                  | Tl <sub>2</sub> S                                     | 440.83   | 8.39                | 448                     | 1367                   | 0.02 <sup>20</sup> aq; s mineral acids         |
| Thiocarbonyl chloride        | S=CCl                                                 | 114.98   | 1.509 <sup>15</sup> |                         | 73.5                   | d aq; s eth                                    |
| Thiocyanogen                 | (SCN) <sub>2</sub>                                    | 116.16   |                     | ca. — 2                 |                        | d aq; s alc, CS <sub>2</sub> , eth             |
| Thionyl, <i>see</i> Sulfenyl |                                                       |          |                     |                         |                        |                                                |
| Thiophosphoryl tribromide    | PSBr <sub>3</sub>                                     | 302.78   | 2.85 <sup>17</sup>  | 38.0                    | 209 d                  | s aq, eth, CS <sub>2</sub>                     |
| trichloride (alpha)          | PSCl <sub>3</sub>                                     | 169.41   | 1.635               | — 40.8                  | 125                    | hyd aq; s bz, chl, CS <sub>2</sub>             |
| trifluoride                  | PSF <sub>3</sub>                                      | 120.03   |                     | — 148.8                 | — 52.2                 |                                                |
| Thiosulfenyl difluoride      | S=SF <sub>2</sub>                                     | 102.13   |                     | — 165                   | — 10.6                 | hyd aq                                         |
| Thorium                      | Th                                                    | 232.038  | 11.7                | 1750                    | 4788                   | s acids                                        |
| chloride                     | ThCl <sub>4</sub>                                     | 373.85   | 4.59                | 770                     | 921                    | s aq, alc                                      |
| fluoride                     | ThF <sub>4</sub>                                      | 308.03   | 6.1                 | 1110                    | 1680                   | s acids                                        |
| iodide                       | ThI <sub>4</sub>                                      | 739.66   | 6.00                | 570                     | 837                    | hyd aq                                         |
| nitrate                      | Th(NO <sub>3</sub> ) <sub>4</sub>                     | 400.06   |                     | d 630, ThO <sub>2</sub> |                        | 191 g/100 mL <sup>20</sup> aq; v s alc         |
| oxide                        | ThO <sub>2</sub>                                      | 264.04   | 10.0                | 3390                    | 4400                   | s hot H <sub>2</sub> SO <sub>4</sub>           |
| sulfate 9-water              | Th(SO <sub>4</sub> ) <sub>2</sub> · 9H <sub>2</sub> O | 586.30   | 2.77                | anhyd 400               |                        | 1.57 g/100 mL <sup>25</sup> aq                 |
| Thullium                     | Tm                                                    | 168.9342 | 9.32                | 1545                    | 1950                   | s acids                                        |
| chloride                     | TmCl <sub>3</sub>                                     | 275.29   |                     | 824                     | 1490                   | s aq, alc                                      |
| fluoride                     | TmF <sub>3</sub>                                      | 225.93   | 7.971               | 1158                    | 2230                   | s H <sub>2</sub> SO <sub>4</sub>               |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                 | Formula                                                        | Formula weight | Density                           | Melting point,<br>°C      | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                          |
|----------------------|----------------------------------------------------------------|----------------|-----------------------------------|---------------------------|----------------------|-----------------------------------------------------------------------------|
| Tin (white)          | Sn                                                             | 118.710        | 7.265                             | 231.928                   | 2602                 | s conc HCl, hot H <sub>2</sub> SO <sub>4</sub>                              |
| (II) acetate         | Sn(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> | 236.80         | 2.31                              | 182.5                     | 240                  | d aq; s dilute HCl                                                          |
| (II) bromide         | SnBr <sub>2</sub>                                              | 278.52         | 5.12                              | 215                       | 639                  | 85 g/100 mL <sup>0</sup> aq; s alc, eth                                     |
| (IV) bromide         | SnBr <sub>4</sub>                                              | 438.33         | 3.34                              | 31                        | 205                  | v a (hyd) aq; s acet, alc                                                   |
| (II) chloride        | SnCl <sub>2</sub>                                              | 189.61         | 3.90                              | 246.9                     | 623                  | 84 g/100 mL <sup>0</sup> aq; s acet, alc, eth                               |
| (IV) chloride        | SnCl <sub>4</sub>                                              | 260.52         | 2.234                             | − 3.3                     | 114.1                | s aq (hyd), alc, acet, bz, eth                                              |
| (II) fluoride        | SnF <sub>2</sub>                                               | 156.71         | 4.57                              | 213                       | 850                  | 30% aq                                                                      |
| (IV) fluoride        | SnF <sub>4</sub>                                               | 194.70         | 4.78                              |                           | subl 705             | hyd aq                                                                      |
| hexafluorozirconate  | Sn[ZrF <sub>6</sub> ]                                          | 323.92         | 4.21                              |                           |                      | s aq                                                                        |
| (II) iodide          | SnI <sub>2</sub>                                               | 372.52         | 5.285                             | 320                       | 714                  | 0.98 <sup>20</sup> aq (d); s bz, chl, alk Cl <sup>−</sup> or I <sup>−</sup> |
| (IV) iodide          | SnI <sub>4</sub>                                               | 626.33         | 4.46                              | 143                       | 364                  | hyd aq; s alc, bz, chl, eth, CCl <sub>4</sub> , CS <sub>2</sub>             |
| (II) oxalate         | SnC <sub>2</sub> O <sub>4</sub>                                | 206.73         | 3.56                              | 280 d                     |                      | s dilute HCl                                                                |
| (II) oxide           | SnO                                                            | 134.71         | 6.45                              | to SnO <sub>2</sub> , 300 |                      | s acids, conc KOH                                                           |
| (IV) oxide           | SnO <sub>2</sub>                                               | 150.71         | 6.95                              | 1630                      |                      | s hot conc KOH (slow)                                                       |
| (II) selenide        | SnSe                                                           | 197.67         | 6.179                             | 861                       |                      | s aqua regia, alkali sulfides                                               |
| (II) sulfate         | SnSO <sub>4</sub>                                              | 214.77         | 4.15                              | to SnO <sub>2</sub> , 378 |                      | 18.9 g/100 mL <sup>20</sup> aq; s dilute H <sub>2</sub> SO <sub>4</sub>     |
| (II) sulfide         | SnS                                                            | 150.78         | 5.08                              | 880                       | 1210                 | s conc HCl, hot conc H <sub>2</sub> SO <sub>4</sub>                         |
| (IV) sulfide         | SnS <sub>2</sub>                                               | 182.84         | 4.5                               | d 600                     |                      | s aq reg, alkali hydroxides & sul-<br>fides                                 |
| (II) telluride       | SnTe                                                           | 246.31         | 6.5                               | 790                       |                      | i aq                                                                        |
| Titanium (hexagonal) | Ti                                                             | 47.867         | 4.506                             | 1668                      | 3287                 | s hot acid, HF                                                              |
| (III) bromide        | TiBr <sub>3</sub>                                              | 287.58         | 4.24                              |                           | subl 794             |                                                                             |
| (IV) bromide         | TiBr <sub>4</sub>                                              | 367.48         | 3.37                              | 39                        | 230                  | hyd aq; 187 g/100 mL abs alc                                                |
| (II) chloride        | TiCl <sub>2</sub>                                              | 118.77         | 3.13                              | 1035                      | 1500                 | d aq; s alc                                                                 |
| (III) chloride       | TiCl <sub>3</sub>                                              | 154.23         | 2.64                              | 425 d                     |                      | s aq (heat evolved), alc                                                    |
| (IV) chloride        | TiCl <sub>4</sub>                                              | 189.68         | 1.73                              | − 25                      | 136.4                | s cold aq, alc                                                              |
| dihydride            | TiH <sub>2</sub>                                               | 49.88          | 3.752                             | d 450                     |                      |                                                                             |
| (IV) fluoride        | TiF <sub>4</sub>                                               | 123.86         | 2.798                             | >400                      | subl 285.5           | s aq (slow hyd); s alc, pyr                                                 |
| (IV) iodide          | TiI <sub>4</sub>                                               | 555.49         | 4.3                               | 150                       | 377                  | s dry nonpolar solvents                                                     |
| (IV) isopropoxide    | Ti[OCH(CH <sub>3</sub> ) <sub>2</sub> ] <sub>4</sub>           | 284.22         | 0.9711 <sup>20</sup> <sub>4</sub> | ~ 20                      | 220                  | d aq; s bz, chl, eth                                                        |
| (II) oxide           | TiO                                                            | 63.87          | 4.95                              | 1750                      | 3660                 | s H <sub>2</sub> SO <sub>4</sub>                                            |

|                            |                                                                                                  |          |       |                                                  |                           |                                                          |
|----------------------------|--------------------------------------------------------------------------------------------------|----------|-------|--------------------------------------------------|---------------------------|----------------------------------------------------------|
| (III) oxide                | Ti <sub>2</sub> O <sub>3</sub>                                                                   | 143.73   | 4.486 | 1842                                             |                           | s H <sub>2</sub> SO <sub>4</sub> , hot HF                |
| (IV) oxide (rutile)        | TiO <sub>2</sub>                                                                                 | 79.87    | 4.23  | 1843                                             |                           | s HF, hot conc H <sub>2</sub> SO <sub>4</sub>            |
| oxide sulfate              | TiOSO <sub>4</sub>                                                                               | 159.94   |       |                                                  |                           | d aq                                                     |
| (III) sulfate              | Ti <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                                                  | 383.93   |       |                                                  |                           | s dilute HCl, dilute H <sub>2</sub> SO <sub>4</sub>      |
| Tungsten                   | W                                                                                                | 183.84   | 19.25 | 3387                                             | 5900                      | s HNO <sub>3</sub> + HF, fusion NaOH + NaNO <sub>3</sub> |
| (V) bromide                | WBr <sub>5</sub>                                                                                 | 583.36   |       | 286                                              | 333                       | hyd aq; s chl, eth                                       |
| (VI) bromide               | WBr <sub>6</sub>                                                                                 | 663.26   | 6.9   | 309                                              | subl 327                  | hyd aq; s eth CS <sub>2</sub>                            |
| (V) chloride               | WCl <sub>5</sub>                                                                                 | 361.10   | 3.875 | 242                                              | 286                       | hyd aq                                                   |
| (VI) chloride              | WCl <sub>6</sub>                                                                                 | 396.56   | 3.52  | 279                                              | 347                       | hyd aq; s CS <sub>2</sub> , CCl <sub>4</sub>             |
| dichloride dioxide         | WCl <sub>2</sub> O <sub>2</sub>                                                                  | 286.74   | 4.67  | 265                                              | d 369                     | hyd aq; s HCl                                            |
| (VI) fluoride              | WF <sub>6</sub>                                                                                  | 297.83   | 3.441 | 2.3                                              | 17.5                      | hyd aq; s anhyd HF                                       |
| (IV) oxide                 | WO <sub>2</sub>                                                                                  | 215.84   | 10.8  | 1550                                             | d 1724                    | s acids, KOH                                             |
| (VI) oxide                 | WO <sub>3</sub>                                                                                  | 231.84   | 7.16  | 1472                                             | 1837                      | i aq; s hot alkali                                       |
| (IV) sulfide               | WS <sub>2</sub>                                                                                  | 247.97   | 7.6   | d 1250                                           |                           | s HNO <sub>3</sub> + HF                                  |
| tetrachloride oxide        | WCl <sub>4</sub> O                                                                               | 341.65   | 11.92 | 211                                              | 227                       | hyd aq                                                   |
| tetrafluoride oxide        | WF <sub>4</sub> O                                                                                | 275.83   | 5.07  | 106                                              | 186                       |                                                          |
| Uranium                    | U                                                                                                | 238.0289 | 19.1  | 1135                                             | 4131                      | s acid                                                   |
| (IV) bromide               | UBr <sub>4</sub>                                                                                 | 557.65   | 5.55  | 519                                              | 777                       | v s aq                                                   |
| (III) chloride             | UCl <sub>3</sub>                                                                                 | 344.39   | 5.51  | 837                                              | 1657                      | v s aq                                                   |
| (IV) chloride              | UCl <sub>4</sub>                                                                                 | 379.84   | 4.725 | 590                                              | 790                       | v s aq (d); s polar org solvents                         |
| (V) chloride               | UCl <sub>5</sub>                                                                                 | 415.29   |       | 287                                              | 527                       | d aq; s CS <sub>2</sub>                                  |
| (VI) chloride              | UCl <sub>6</sub>                                                                                 | 450.75   | 3.6   | 177                                              | 392                       | hyd aq; s chl                                            |
| (IV) fluoride              | UF <sub>4</sub>                                                                                  | 314.02   | 6.70  | 1036                                             | 1417                      | s conc acids (d); alk (d)                                |
| (VI) fluoride              | UF <sub>6</sub>                                                                                  | 352.02   | 5.09  | 64.0                                             | subl 56.5                 | hyd aq; s chl, CCl <sub>4</sub>                          |
| (III) hydride              | UH <sub>3</sub>                                                                                  | 241.05   | 11.1  |                                                  |                           | i aq                                                     |
| (IV) iodide                | UI <sub>4</sub>                                                                                  | 745.65   | 5.6   | 506                                              | 757                       | s aq                                                     |
| (IV) oxide (pitchblende)   | UO <sub>2</sub>                                                                                  | 270.03   | 10.97 | 2827                                             |                           | s conc HNO <sub>3</sub>                                  |
| (VI) oxide                 | UO <sub>3</sub>                                                                                  | 286.03   | 7.29  | d 1300                                           |                           | i aq; s HCl, HNO <sub>3</sub>                            |
| octaoxide [(V,VI) oxide]   | U <sub>3</sub> O <sub>8</sub>                                                                    | 842.08   | 8.38  | d 1300 to UO <sub>2</sub>                        |                           | s HNO <sub>3</sub>                                       |
| peroxide 2-water           | UO <sub>4</sub> ·2H <sub>2</sub> O                                                               | 338.06   |       | d 90–195 to U <sub>2</sub> O <sub>7</sub> (slow) | d >200 to UO <sub>2</sub> | d by HCl                                                 |
| Uranyl(VI) acetate 2-water | UO <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 2H <sub>2</sub> O | 422.13   | 2.893 | anhyd 110                                        | d 275                     | 7.7 g/100 mL <sup>15</sup> aq; sl s alc                  |
| chloride                   | UO <sub>2</sub> Cl <sub>2</sub>                                                                  | 340.93   | 5.43  | 577                                              |                           | 320 g/100 mL <sup>18</sup> aq; s acet, alc               |
| fluoride                   | UO <sub>2</sub> F <sub>2</sub>                                                                   | 308.03   | 6.37  | d 300                                            |                           | v s aq                                                   |
| nitrate 6-water            | UO <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                              | 502.13   | 2.807 | 60                                               | d 118                     | 155 g/100 mL <sup>20</sup> aq; v s alc, eth              |
| sulfate 3-water            | UO <sub>2</sub> SO <sub>4</sub> · 3H <sub>2</sub> O                                              | 420.14   | 3.28  | d 100                                            |                           | g/100 mL: 21 aq, 4 alc                                   |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| 3.58      | Name                   | Formula                                                             | Formula weight | Density            | Melting point,<br>°C        | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                   |
|-----------|------------------------|---------------------------------------------------------------------|----------------|--------------------|-----------------------------|----------------------|----------------------------------------------------------------------|
|           |                        |                                                                     |                |                    |                             |                      |                                                                      |
| 3.58      | Vanadium               | V                                                                   | 50.9415        | 6.11 <sup>19</sup> | 1917                        | 3421                 | s HF, HNO <sub>3</sub> , hot H <sub>2</sub> SO <sub>4</sub> , aq reg |
|           | (IV) chloride          | VCl <sub>4</sub>                                                    | 192.75         | 1.82               | − 25.7                      | 148                  | hyd aq; s nonpolar solvents                                          |
|           | dichloride oxide       | VCl <sub>2</sub> O                                                  | 137.86         | 2.88               | disprop 384                 |                      | hyd (slow) aq; s abs alc, HOAc                                       |
|           | (III) fluoride         | VF <sub>3</sub>                                                     | 107.94         | 3.363              | ≈ 1400                      | subl 800             | i almost all organic solvents                                        |
|           | (IV) fluoride          | VF <sub>4</sub>                                                     | 126.94         | 3.15               | subl 120 (vac)<br>& disprop |                      | s aq, acet, HOAc                                                     |
|           | (V) fluoride           | VF <sub>5</sub>                                                     | 145.93         | 2.50               | 19.5                        | 48                   | hyd aq; v s anhyd HF, acet, alc                                      |
|           | (II) oxide             | VO                                                                  | 66.94          | 5.76               | 1790                        |                      | s HCl                                                                |
|           | (III) oxide            | V <sub>2</sub> O <sub>3</sub>                                       | 149.88         | 4.87               | 1940                        |                      | sl s acids                                                           |
|           | (IV) oxide             | VO <sub>2</sub>                                                     | 82.94          | 4.34               | 1967                        |                      | s acids, alkalis                                                     |
|           | (V) oxide              | V <sub>2</sub> O <sub>5</sub>                                       | 181.88         | 3.35               | 670                         | d 1800               | 0.07 aq; s conc acids, alkalis                                       |
|           | (IV) oxide sulfate     | VOSO <sub>4</sub>                                                   | 163.00         |                    |                             |                      | s aq                                                                 |
|           | (III) sulfate          | V <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                      | 390.07         |                    | 410 (vac)                   |                      | s (slow) aq, HNO <sub>3</sub>                                        |
|           | (III) sulfide          | V <sub>2</sub> S <sub>3</sub>                                       | 198.08         | 4.72               | d 600                       |                      | s hot acids, alkali sulfides                                         |
|           | Xenon                  | Xe                                                                  | 131.29         | 5.761 g/L          | − 111.8                     | − 108.04             | 10.8 mL/100 mL <sup>20</sup> aq                                      |
|           | difluoride             | XeF                                                                 | 169.29         | 4.32               | 129.0                       | subl 114.3           | 2.5 g/100 mL <sup>0</sup> aq                                         |
|           | hexafluoride           | XeF <sub>6</sub>                                                    | 245.28         | 3.56               | 49.5                        | 75.6                 | hyd aq                                                               |
|           | tetrafluoride          | XeF <sub>4</sub>                                                    | 207.28         | 4.04               | 117.1                       | subl 115.7           | hyd aq; s F <sub>3</sub> CCOOH                                       |
|           | trioxide               | XeO <sub>3</sub>                                                    | 179.29         | 4.55               | explodes 25                 |                      | s aq giving xenic acid                                               |
| Ytterbium | Ytterbium              | Yb                                                                  | 173.04         | 6.90               | 819                         | 1196                 | s acids                                                              |
|           | (II) chloride          | YbCl <sub>2</sub>                                                   | 243.95         | 5.27               | 721                         | 1930                 | s aq                                                                 |
|           | (III) chloride 6-water | YbCl <sub>3</sub> · 6H <sub>2</sub> O                               | 387.49         | 2.57               | anhyd 180                   | mp: 865              | v s aq                                                               |
|           | (III) fluoride         | YbF <sub>3</sub>                                                    | 230.04         | 8.17               | 1157                        | 2230                 | s H <sub>2</sub> SO <sub>4</sub>                                     |
|           | (III) nitrate 4-water  | Yb(NO <sub>3</sub> ) <sub>3</sub> · 4H <sub>2</sub> O               | 431.12         |                    |                             |                      | s aq                                                                 |
|           | (III) oxide            | Yb <sub>2</sub> O <sub>3</sub>                                      | 394.08         | 9.18               | 2435                        |                      | s dilute acids                                                       |
|           | (III) sulfate 8-water  | Yb <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O | 778.39         | 3.3                |                             |                      | 34.8 g/100 mL <sup>20</sup> aq                                       |
|           | Yttrium                | Y                                                                   | 88.9059        | 4.472              | 1522                        | 3345                 | s hot water (d)                                                      |
| Yttrium   | chloride               | YCl <sub>3</sub>                                                    | 195.26         | 2.61               | 721                         | 1510                 | 79 g/100 mL <sup>20</sup> aq; s alc                                  |
|           | fluoride               | YF <sub>3</sub>                                                     | 145.90         | 4.0                | 1152                        | 2230                 | s conc acids (d)                                                     |

|                                |                                                                                     |        |       |                              |              |                                                          |
|--------------------------------|-------------------------------------------------------------------------------------|--------|-------|------------------------------|--------------|----------------------------------------------------------|
| nitrate 6-water<br>oxide       | $\text{Y}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$                                 | 383.01 | 2.68  | $-3\text{H}_2\text{O}$ , 100 |              | 171 g/100 mL <sup>20</sup> aq                            |
|                                | $\text{Y}_2\text{O}_3$                                                              | 225.81 | 5.03  | 2440                         | 4300         | s acids                                                  |
| sulfate 8-water                | $\text{Y}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$                               | 610.12 | 2.56  | anhyd 400                    | d > 1000     | 9.6 g/100 mL <sup>20</sup> aq                            |
|                                | Zn                                                                                  | 65.39  | 7.14  | 419.527                      | 907          | i aq; s acids, alkalis (slow)                            |
| acetate dihydrate              | $\text{Zn}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 2\text{H}_2\text{O}$             | 219.51 | 1.735 | 237 d                        |              | g/100 mL: 41.6 <sup>20</sup> aq, 3.3 alc                 |
| arsenate(III)(1-)              | $\text{Zn}(\text{AsO}_2)_2$                                                         | 279.23 |       |                              |              | s acids                                                  |
| arsenate(V)(3-) 8-water        | $\text{Zn}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$                             | 618.13 | 3.33  |                              |              | s acids and alkalis                                      |
| bromide                        | $\text{ZnBr}_2$                                                                     | 225.20 | 4.5   | 394                          | 697          | g/100 mL: 471 <sup>25</sup> aq, 200 alc; s<br>KOH, eth   |
| carbonate                      | $\text{ZnCO}_3$                                                                     | 125.40 | 4.4   | $-\text{CO}_2$ , 300         |              | 0.02 <sup>25</sup> aq; s acids, KOH, $\text{NH}_4$ salts |
| chloride                       | $\text{ZnCl}_2$                                                                     | 136.29 | 2.907 | 290                          | 732          | g/100 ml: 395 <sup>20</sup> aq, 77 alc, 50 gly; v s acet |
| chromate(VI)                   | $\text{ZnCrO}_4$                                                                    | 181.39 | 3.40  |                              |              | s acids                                                  |
| cyanide                        | $\text{Zn}(\text{CN})_2$                                                            | 117.43 | 1.852 | d 800                        |              | 0.058 <sup>18</sup> aq; s acids, KCN, KOH                |
| fluoride                       | $\text{ZnF}_2$                                                                      | 103.39 | 4.9   | 872                          | 1500         | s $\text{HNO}_3$ , HCl, $\text{NH}_4\text{OH}$           |
| hexafluorosilicate 6-water     | $\text{Zn}[\text{SiF}_6] \cdot 6\text{H}_2\text{O}$                                 | 315.56 | 2.104 | d 100                        |              | v s aq                                                   |
| iodate                         | $\text{Zn}(\text{IO}_3)_2$                                                          | 415.20 | 5.063 | d                            |              | 0.87 <sup>20</sup> aq; s $\text{HNO}_3$ , KOH            |
| iodide                         | $\text{ZnI}_2$                                                                      | 319.20 | 4.74  | 446                          | 625 d        | g/100 mL: 332 <sup>20</sup> aq, 50 gly; v s alc          |
| nitrate 6-water                | $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$                                | 297.49 | 2.067 | $-6\text{H}_2\text{O}$ , 131 |              | 146 g/100 mL <sup>0</sup> aq; v s alc                    |
| oxide                          | $\text{ZnO}$                                                                        | 81.39  | 5.60  | 1975                         |              | i aq; s acids, KOH, $\text{NH}_4\text{OH}$               |
| peroxide                       | $\text{ZnO}_2$                                                                      | 97.39  | 1.57  | d > 150                      | explodes 212 | d (slow) aq; s dilute acids (d)                          |
| 1,4-phenolsulfonate<br>8-water | $\text{Zn}[\text{C}_6\text{H}_4(\text{OH})\text{SO}_3]_2 \cdot 8\text{H}_2\text{O}$ | 555.84 |       | anhyd 120                    |              | g/100 mL: 63 aq, 56 alc                                  |
| phosphate(V)                   | $\text{Zn}_3(\text{PO}_4)_2$                                                        | 386.11 | 3.998 | 900                          |              | s acids, $\text{NH}_4\text{OH}$                          |
| phosphide                      | $\text{Zn}_3\text{P}_2$                                                             | 258.12 | 4.55  | 420                          | 1100         | d aq, HCl (viol); s bz, $\text{CS}_2$                    |
| propionate                     | $\text{Zn}(\text{C}_3\text{H}_5\text{O}_2)_2$                                       | 211.53 |       |                              |              | 32% <sup>15</sup> aq; 2.8% <sup>15</sup> alc             |
| selenide                       | $\text{ZnSe}$                                                                       | 144.35 | 5.65  | > 1100                       |              | d dilute $\text{HNO}_3$                                  |
| silicate(2-)                   | $\text{Zn}_2\text{SiO}_4$                                                           | 222.86 | 4.10  | 1512                         |              | i aq or dilute acids                                     |
| stearate                       | $\text{Zn}(\text{C}_{18}\text{H}_{35}\text{O}_2)_2$                                 | 632.34 | 1.095 | 130                          |              | d dil acids; s bz; i aq, alc, eth                        |
| sulfate                        | $\text{ZnSO}_4$                                                                     | 161.45 | 3.8   | 680 d                        |              | 53.8% <sup>20</sup> aq                                   |
| sulfate 7-water                | $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$                                           | 287.56 | 1.97  | anhyd 280                    | d > 500      | g/100 mL: 167 aq, 40 gly; i alc                          |
| sulfide (wurzite)              | $\text{ZnS}$                                                                        | 97.46  | 4.09  | 1722                         |              | i aq; s dilute mineral acids                             |
| telluride                      | $\text{ZnTe}$                                                                       | 192.99 | 6.34  | 1239                         |              | d (slow) aq or dilute HCl                                |
| thiocyanate                    | $\text{Zn}(\text{SCN})_2$                                                           | 181.56 |       |                              |              | 0.14 aq; s alc                                           |

**TABLE 3.2** Physical Constants of Inorganic Compounds (*Continued*)

| Name                     | Formula                                               | Formula weight | Density | Melting point,<br>°C                          | Boiling point,<br>°C | Solubility in<br>100 parts solvent                                                    |
|--------------------------|-------------------------------------------------------|----------------|---------|-----------------------------------------------|----------------------|---------------------------------------------------------------------------------------|
| Zirconium                | Zr                                                    | 91.224         | 6.52    | 1852                                          | 3577                 | s aq reg, HF, hot H <sub>3</sub> PO <sub>4</sub> , fusion with KOH + KNO <sub>3</sub> |
| (IV) bromide             | ZrBr <sub>4</sub>                                     | 410.84         | 3.98    | 450                                           | subl 357             |                                                                                       |
| carbide                  | ZrC                                                   | 103.23         | 6.73    | 3532                                          | 5100                 | sl s conc H <sub>2</sub> SO <sub>4</sub>                                              |
| (II) chloride            | ZrCl <sub>2</sub>                                     | 162.13         | 3.6     | 727                                           | 1292                 | d aq                                                                                  |
| (IV) chloride            | ZrCl <sub>4</sub>                                     | 233.03         | 2.80    | 437 (25 atm)                                  | subl 334             | hyd aq to ZrCl <sub>2</sub> O; s alc, eth                                             |
| diboride                 | ZrB <sub>2</sub>                                      | 112.85         | 6.17    | 3245                                          | d 4193               |                                                                                       |
| dichloride oxide 8-water | ZrCl <sub>2</sub> O · 8H <sub>2</sub> O               | 322.25         | 1.91    | anhyd 210                                     | d 410                | v s aq, alc                                                                           |
| dihydride                | ZrH <sub>2</sub>                                      | 93.24          | 5.61    |                                               |                      | i aq                                                                                  |
| (IV) fluoride            | ZrF <sub>4</sub>                                      | 167.22         | 4.436   | 932 <sup>mp</sup>                             | subl 912             | 1.32 g/100 mL <sup>20</sup> aq                                                        |
| (IV) hydroxide           | Zr(OH) <sub>4</sub>                                   | 159.25         | 3.25    | to ZrO <sub>2</sub> , 500                     |                      | s mineral acids                                                                       |
| (IV) iodide              | ZrI <sub>4</sub>                                      | 598.84         |         | 499 (sealed tube)                             | subl 432.5           | s aq (d), eth                                                                         |
| (IV) nitrate 5-water     | Zr(NO <sub>3</sub> ) <sub>4</sub> · 5H <sub>2</sub> O | 429.32         |         | d 100                                         |                      | v s aq; s alc                                                                         |
| (IV) oxide               | ZrO <sub>2</sub>                                      | 123.22         | 5.68    | 2678                                          | 4300                 | s hot H <sub>2</sub> SO <sub>4</sub> , HF (slow)                                      |
| (IV) silicate(4—)        | ZrSiO <sub>4</sub>                                    | 183.31         | 4.56    | d 1540 to ZrO <sub>2</sub> + SiO <sub>2</sub> |                      | unaffected by aqueous reagents                                                        |
| sulfate 4-water          | Zr(SO <sub>4</sub> ) <sub>2</sub> · 4H <sub>2</sub> O | 355.41         | 2.80    | anhyd 380                                     |                      | 52.5 g/100 g aqueous solution                                                         |

**TABLE 3.3** Synonyms and Mineral Names

---

|                                                            |                                                         |
|------------------------------------------------------------|---------------------------------------------------------|
| Acanthite, <i>see</i> Silver sulfide                       | Cementite, <i>see</i> tri-Iron carbide                  |
| Alabandite, <i>see</i> Manganese sulfide                   | Cerargyrite, <i>see</i> Silver chloride                 |
| Alamosite, <i>see</i> Lead(II) silicate(2-)                | Cerussite, <i>see</i> Lead carbonate                    |
| Altaite, <i>see</i> Lead telluride                         | Chalcanthite, <i>see</i> Copper(II) sulfate 5-water     |
| Alumina, <i>see</i> Aluminum oxide                         | Chalcocite, <i>see</i> Copper(I) sulfide                |
| Alundum, <i>see</i> Aluminum oxide                         | Chalk, <i>see</i> Calcium carbonate                     |
| Alunogenite, <i>see</i> Aluminum sulfate 18-water          | Chile nitre, <i>see</i> Sodium nitrate                  |
| Amphibole, <i>see</i> Magnesium silicate(2-)               | Chile saltpeter, <i>see</i> Sodium nitrate              |
| Andalusite, <i>see</i> Aluminum silicon oxide (1/1)        | Chloromagnesite, <i>see</i> Magnesium chloride          |
| Anglesite, <i>see</i> Lead sulfate                         | Chlorosulfonic acid, <i>see</i> Hydrogen chlorosulfate  |
| Anhydrite, <i>see</i> Calcium sulfate                      | Cinnabar, <i>see</i> Mercury(II) sulfide                |
| Anhydronite, <i>see</i> Magnesium perchlorate              | Claudetite, <i>see</i> Arsenic(III) oxide dimer         |
| Aragonite, <i>see</i> Calcium carbonate                    | Clausthalite, <i>see</i> Lead selenide                  |
| Arcanite, <i>see</i> Potassium sulfate                     | Clinoenstatite, <i>see</i> Magnesium silicate(2-)       |
| Argentite, <i>see</i> Silver sulfide                       | Columbium, <i>see</i> under Niobium                     |
| Argol, <i>see</i> Potassium hydrogen tartrate              | Corrosive sublimate, <i>see</i> Mercury(II) chloride    |
| Arkansite, <i>see</i> Titanium(IV) oxide                   | Corundum, <i>see</i> Aluminum oxide                     |
| Arsenolite, <i>see</i> Arsenic(III) oxide dimer            | Cotunite, <i>see</i> Lead chloride                      |
| Arsine, <i>see</i> Arsenic hydride                         | Covellite, <i>see</i> Copper(II) sulfide                |
| Auric and aurous, <i>see</i> under Gold                    | Cream of tartar, <i>see</i> Potassium hydrogen tartrate |
| Azoimide, <i>see</i> Hydrogen azide                        | Crocoite, <i>see</i> Lead chromate(VI)(2-)              |
| Azurite, <i>see</i> Copper(II) carbonate—dihydroxide (2/1) | Cryolite, <i>see</i> Sodium hexafluoroaluminate         |
|                                                            | Cryptohalite, <i>see</i> Ammonium hexafluorosilicate    |
|                                                            | Cupric and cuprous, <i>see</i> under Copper             |
|                                                            | Cuprite, <i>see</i> Copper(I) oxide                     |
| Baddeleyite, <i>see</i> Zirconium(IV) oxide                |                                                         |
| Baking soda, <i>see</i> Sodium hydrogen carbonate          | Dakin's solution, <i>see</i> Sodium hypochlorite        |
| Barite (barytes), <i>see</i> Barium sulfate                | Dehydrite, <i>see</i> Magnesium perchlorate             |
| Bieberite, <i>see</i> Cobalt sulfate 7-water               | Dental gas, <i>see</i> Nitrogen(I) oxide                |
| Bismuthine, <i>see</i> Bismuth hydride                     | Diamond, <i>see</i> Carbon                              |
| Bismuthinite, <i>see</i> Bismuth sulfide                   | Dichlorodisulfane, <i>see</i> di-Sulfur dichloride      |
| Bleaching powder, <i>see</i> Calcium hydrochlorite         | Diuretic salt, <i>see</i> Potassium acetate             |
| Bleaching solution, <i>see</i> Sodium hydrochlorite        | Dolomite, <i>see</i> Calcium magnesium carbonate (1/1)  |
| Blue coppers, <i>see</i> Copper(II) sulfate 7-water        | Dry ice, <i>see</i> Carbon dioxide (solid)              |
| Boracic acid, <i>see</i> Hydrogen borate                   |                                                         |
| Borax, <i>see</i> Sodium tetraborate 10-water              | Enstatite, <i>see</i> Magnesium silicate(2-)            |
| Braunite, <i>see</i> Manganese(III) oxide                  | Epsom salts, <i>see</i> Magnesium sulfate 7-water       |
| Brimstone, <i>see</i> Sulfur                               | Epsomite, <i>see</i> Magnesium sulfate 7-water          |
| Bromellite, <i>see</i> Beryllium oxide                     | Eriochalcite, <i>see</i> Copper(II) chloride            |
| Bromosulfonic acid, <i>see</i> Hydrogen bromosulfate       |                                                         |
| Bromyrite, <i>see</i> Silver bromide                       | Fayalite, <i>see</i> Iron(II) silicate(4-)              |
| Brookite, <i>see</i> Titanium(IV) oxide                    | Ferric and ferrous, <i>see</i> under Iron               |
| Brucite, <i>see</i> Magnesium hydroxide                    | Fluorine oxide, <i>see</i> Oxygen difluoride            |
| Bunsenite, <i>see</i> Nickel oxide                         | Fluoristan, <i>see</i> Tin(II) fluoride                 |
|                                                            | Fluorite, <i>see</i> Calcium fluoride                   |
| Cacodylate, <i>see</i> Sodium dimethylarsenate 3-water     | Fluorosulfonic acid, <i>see</i> Hydrogen fluorosulfate  |
| Caesium, <i>see</i> under Cesium                           | Fluorspar, <i>see</i> Calcium fluoride                  |
| Calamine, <i>see</i> Zinc carbonate                        | Forsterite, <i>see</i> Magnesium silicate(4-)           |
| Calcia, <i>see</i> Calcium oxide                           | Freezing salt, <i>see</i> Sodium chloride               |
| Calcite, <i>see</i> Calcium carbonate                      | Fulminating mercury, <i>see</i> Mercury fulminate       |
| Calomel, <i>see</i> Mercury(I) chloride                    |                                                         |
| Caro's acid, <i>see</i> Hydrogen peroxosulfate             | Galena, <i>see</i> Lead sulfite                         |
| Cassiopeium, <i>see</i> Lutetium                           | Glauber's salt, <i>see</i> Sodium sulfate 10-water      |
| Cassiterite, <i>see</i> Tin(IV) oxide                      | Goethite, <i>see</i> Iron(II) hydroxide oxide           |
| Caustic potash, <i>see</i> Potassium hydroxide             | Goslarite, <i>see</i> Zinc sulfate 7-water              |
| Caustic soda, <i>see</i> Sodium hydroxide                  | Graham's salt, <i>see</i> Sodium phosphate(1-)          |
| Celestite, <i>see</i> Strontium sulfate                    | Graphite, <i>see</i> Carbon                             |

---

**TABLE 3.3** Synonyms and Mineral Names (*Continued*)

---

|                                                                                     |                                                                       |
|-------------------------------------------------------------------------------------|-----------------------------------------------------------------------|
| Greenockite, <i>see</i> Cadmium sulfide                                             | Moissanite, <i>see</i> Silicon carbide                                |
| Gruenerite, <i>see</i> Iron(II) silicate(2-)                                        | Molybdenite, <i>see</i> Molybdenum disulfide                          |
| Guanajuatite, <i>see</i> Bismuth selenide                                           | Molybdate, <i>see</i> Molybdenum(VI) oxide                            |
| Gypsum, <i>see</i> Calcium sulfate 2-water                                          | Molysite, <i>see</i> Iron(III) chloride                               |
| Halite, <i>see</i> Sodium chloride                                                  | Montroydite, <i>see</i> Mercury(II) oxide                             |
| Hausmannite, <i>see</i> Manganese(II,IV) oxide                                      | Morenosite, <i>see</i> Nickel sulfate 7-water                         |
| Heavy hydrogen, <i>see</i> Hydrogen[ <sup>2</sup> H] or name followed by - <i>d</i> | Mosaic gold, <i>see</i> Tin disulfide                                 |
| Heavy water, <i>see</i> Hydrogen[ <sup>2</sup> H] oxide                             | Muriatic acid, <i>see</i> Hydrogen chloride, aqueous solutions        |
| Heazlewoodite, <i>see</i> <i>tri</i> -Nickel disulfide                              | Nantokite, <i>see</i> Copper(I) chloride                              |
| Hematite, <i>see</i> Iron(III) oxide                                                | Natron, <i>see</i> Sodium carbonate                                   |
| Hermannite, <i>see</i> Manganese silicate                                           | Naumannite, <i>see</i> Silver selenide                                |
| Hessite, <i>see</i> Silver telluride                                                | Neutral verdigris, <i>see</i> Copper(II) acetate                      |
| Hieratite, <i>see</i> Potassium hexafluorosilicate                                  | Nitre (niter), <i>see</i> Potassium nitrate                           |
| Hydroazotic acid, <i>see</i> Hydrogen azide                                         | Nitric oxide, <i>see</i> Nitrogen(II) oxide                           |
| Hydrophilite, <i>see</i> Calcium chloride                                           | Nitrobarite, <i>see</i> Barium nitrate                                |
| Hydrosulfite, <i>see</i> Sodium dithionate(III)                                     | Nitromagnesite, <i>see</i> Magnesium nitrate 6-water                  |
| Hypo (photographic), <i>see</i> Sodium thiosulfate 5-water                          | Nitroprusside, <i>see</i> Sodium pentacyanonitrosylferate(II) 2-water |
| Hypophosphite, <i>see</i> under Phosphinate                                         | Oldhamite, <i>see</i> Calcium sulfide                                 |
| Ice, <i>see</i> Hydrogen oxide (solid)                                              | Opal, <i>see</i> Silicon dioxide                                      |
| Iceland spar, <i>see</i> Calcium carbonate                                          | Orpiment, <i>see</i> Arsenic trisulfide                               |
| Iodyrite, <i>see</i> Silver iodide                                                  | Oxygen powder, <i>see</i> Sodium peroxide                             |
| Jeweler's borax, <i>see</i> Sodium tetraborate 10-water                             | Paris green, <i>see</i> Copper acetate arsenate(III) (1/3)            |
| Jeweler's rouge, <i>see</i> Iron(III) oxide                                         | Pawellite, <i>see</i> Calcium molybdate(VI)(2-)                       |
| Kalinite, <i>see</i> Aluminum potassium bis(sulfate)                                | Pearl ash, <i>see</i> Potassium carbonate                             |
| Kernite, <i>see</i> Sodium tetraborate                                              | Perborax, <i>see</i> Sodium peroxoborate                              |
| Kyanite, <i>see</i> Aluminum silicon oxide (1/1)                                    | Periclase, <i>see</i> Magnesium oxide                                 |
| Laughing gas, <i>see</i> Nitrogen(I) oxide                                          | Persulfate, <i>see</i> Peroxodisulfate                                |
| Lautarite, <i>see</i> Calcium iodate                                                | Phosgene, <i>see</i> Carbonyl chloride                                |
| Lawrencite, <i>see</i> Iron(II) chloride                                            | Phosphine, <i>see</i> Hydrogen phosphide                              |
| Lechatelierite, <i>see</i> Silicon dioxide                                          | Pickling acid, <i>see</i> Hydrogen sulfate                            |
| Lime, <i>see</i> Calcium oxide                                                      | Pitchblende, <i>see</i> Uranium(IV) oxide                             |
| Litharge, <i>see</i> Lead(II) oxide                                                 | Plaster of Paris, <i>see</i> Calcium sulfate hemihydrate              |
| Lithium aluminum hydride, <i>see</i> Lithium tetrahydridoaluminate                  | Plattnerite, <i>see</i> Lead(IV) oxide                                |
| Lodestone, <i>see</i> Iron(II,III) oxide                                            | Polianite, <i>see</i> Manganese(IV) oxide                             |
| Lunar caustic, <i>see</i> Silver nitrate                                            | Polishing powder, <i>see</i> Silicon dioxide                          |
| Lye, <i>see</i> Sodium hydroxide                                                    | Potash, <i>see</i> Potassium carbonate                                |
| Magnesia, <i>see</i> Magnesium oxide                                                | Potassium acid phthalate, <i>see</i> Potassium hydrogen phthalate     |
| Magnesite, <i>see</i> Magnesium carbonate                                           | Prussic acid, <i>see</i> Hydrogen cyanide                             |
| Magnetite, <i>see</i> Iron(II,III) oxide                                            | Pyrite, <i>see</i> Iron disulfide                                     |
| Malachite, <i>see</i> Copper carbonate dihydroxide                                  | Pyrochroite, <i>see</i> Manganese(II) hydroxide                       |
| Manganosite, <i>see</i> Manganese(II) oxide                                         | Pyrohyttophosphite, <i>see</i> diphosphate(IV)                        |
| Marcasite, <i>see</i> Iron disulfide                                                | Pyrolusite, <i>see</i> Manganese(IV) oxide                            |
| Marshite, <i>see</i> Copper(I) iodide                                               | Pyrophanite, <i>see</i> Manganese titanate(IV)(2-)                    |
| Mascagnite, <i>see</i> Ammonium sulfate                                             | Pyrophosphate, <i>see</i> Diphosphate(V)                              |
| Massicotite, <i>see</i> Lead oxide                                                  | Pyrosulfuric acid, <i>see</i> Hydrogen disulfate                      |
| Mercuric and mercurous, <i>see</i> under Mercury                                    | Quartz, <i>see</i> Silicon dioxide                                    |
| Metacinnabar, <i>see</i> Mercury(II) sulfide                                        | Quicksilver, <i>see</i> Mercury                                       |
| Millerite, <i>see</i> Nickel sulfide                                                | Realgar, <i>see</i> di-Arsenic disulfide                              |
| Mirabilite, <i>see</i> Sodium sulfate                                               | Red lead, <i>see</i> Lead(II,IV) oxide                                |
| Mohr's salt, <i>see</i> Ammonium iron(II) sulfate 6-water                           | Rhodochrosite, <i>see</i> Manganese carbonate                         |

---



**TABLE 3.3** Synonyms and Mineral Names (*Continued*)

---

|                                                                              |                                                                 |
|------------------------------------------------------------------------------|-----------------------------------------------------------------|
| Rhodonite, <i>see</i> Manganese silicate(1–)                                 | Sylvite, <i>see</i> Potassium chloride                          |
| Rochelle salt, <i>see</i> Potassium sodium tartrate 4-water                  | Szmkite, <i>see</i> Manganese(II) sulfate hydrate               |
| Rock crystal, <i>see</i> Silicon dioxide                                     | Tarapacaite, <i>see</i> Potassium chromate(VI)                  |
| Rutile, <i>see</i> Titanium(IV) oxide                                        | Tellurite, <i>see</i> Tellurium dioxide                         |
| Sal soda, <i>see</i> Sodium carbonate 10-water                               | Tenorite, <i>see</i> Copper(II) oxide                           |
| Saltpeter, <i>see</i> Potassium nitrate                                      | Tephroite, <i>see</i> Manganese silicate(1–)                    |
| Scacchite, <i>see</i> Manganese chloride                                     | Thenardite, <i>see</i> Sodium sulfate                           |
| Scheelite, <i>see</i> Calcium tungstate(VI)(2–)                              | Thionyl, <i>see</i> Sulfanyl                                    |
| Sellaite, <i>see</i> Magnesium fluoride                                      | Thorianite, <i>see</i> Thorium dioxide                          |
| Senarmontite, <i>see</i> Antimony(III) oxide                                 | Topaz, <i>see</i> Aluminum hexafluorosilicate                   |
| Siderite, <i>see</i> Iron(II) carbonate                                      | Tridymite, <i>see</i> Silicon dioxide                           |
| Siderotil, <i>see</i> Iron(II) sulfate 5-water                               | Troilite, <i>see</i> Iron(II) sulfide                           |
| Silica, <i>see</i> Silicon dioxide                                           | Trona, <i>see</i> Sodium carbonate—hydrogen carbonate dihydrate |
| Silicotungstic acid, <i>see</i> Silicon oxide—tungsten oxide—water (1/12/26) | Tschemigite, <i>see</i> Aluminum ammonium bis(sulfate)          |
| Sillimanite, <i>see</i> Aluminum silicon oxide (1/1)                         | Tungstenite, <i>see</i> Tungsten disulfide                      |
| Smithsonite, <i>see</i> Zinc carbonate                                       | Tungstite, <i>see</i> Hydrogen tungstate                        |
| Soda ash, <i>see</i> Sodium carbonate                                        | Uraninite, <i>see</i> Uranium(IV) oxide                         |
| Spelter, <i>see</i> Zinc metal                                               | Valentinite, <i>see</i> Antimony(III) oxide                     |
| Sphalerite, <i>see</i> Zinc sulfide                                          | Verdigris, <i>see</i> Copper acetate hydrate                    |
| Spherochalcite, <i>see</i> Cobalt(II) carbonate                              | Vermillion, <i>see</i> Mercury(II) sulfide                      |
| Spinel, <i>see</i> Magnesium aluminate(2–)                                   | Villiaumite, <i>see</i> Sodium fluoride                         |
| Stannic and stannous, <i>see</i> under Tin                                   | Vitamin B <sub>3</sub> , <i>see</i> Calcium (+)pantothenate     |
| Stibine, <i>see</i> Antimony hydride                                         | Washing soda, <i>see</i> Sodium carbonate 10-water              |
| Stibnite, <i>see</i> Antimony(III) sulfide                                   | Whitlockite, <i>see</i> Calcium phosphate                       |
| Stolzite, <i>see</i> Lead tungstate(VI)(2–)                                  | Willemite, <i>see</i> Zinc silicate(4–)                         |
| Strengite, <i>see</i> Iron(III) phosphate                                    | Wolfram, <i>see</i> Tungsten                                    |
| Strontianite, <i>see</i> Strontium carbonate                                 | Wuestite, <i>see</i> Iron(II) oxide                             |
| Sugar of lead, <i>see</i> Lead acetate                                       | Wulfenite, <i>see</i> Lead molybdate(VI)(2–)                    |
| Sulfamate, <i>see</i> Amidosulfate                                           | Wurtzite, <i>see</i> Zinc sulfide                               |
| Sulphate, <i>see</i> Sulfate                                                 | Zincite, <i>see</i> Zinc oxide                                  |
| Sulfurated lime, <i>see</i> Calcium sulfide                                  | Zincosite, <i>see</i> Zinc sulfate                              |
| Sulfuretted hydrogen, <i>see</i> Hydrogen sulfide                            | Zincspar, <i>see</i> Zinc carbonate                             |
| Sulphur, <i>see</i> Sulfur                                                   | Zirconia, <i>see</i> Zirconium oxide                            |
| Sulfuryl, <i>see</i> Sulfonyl                                                |                                                                 |
| Sycoporite, <i>see</i> Cobalt sulfide                                        |                                                                 |

---

---

# SECTION 4

---

## PROPERTIES OF ATOMS, RADICALS, AND BONDS

---

|              |                                                                    |             |
|--------------|--------------------------------------------------------------------|-------------|
| <b>4.1</b>   | <b>ELEMENTS</b>                                                    | <b>4.1</b>  |
|              | Table 4.1 Electronic Configuration and Properties of the Elements  | 4.2         |
| <b>4.2</b>   | <b>IONIZATION ENERGY</b>                                           | <b>4.6</b>  |
|              | Table 4.2 Ionization Energy of the Elements                        | 4.6         |
|              | Table 4.3 Ionization Energy of Molecular and Radical Species       | 4.8         |
| <b>4.3</b>   | <b>ELECTRON AFFINITY</b>                                           | <b>4.24</b> |
|              | Table 4.4 Electron Affinities of Elements, Molecules, and Radicals | 4.24        |
| <b>4.4</b>   | <b>ELECTRONEGATIVITY</b>                                           | <b>4.28</b> |
|              | Table 4.5 Electronegativities of the Elements                      | 4.29        |
| <b>4.5</b>   | <b>BOND LENGTHS AND STRENGTHS</b>                                  | <b>4.29</b> |
| <b>4.5.1</b> | <b>Atom Radius</b>                                                 | <b>4.29</b> |
|              | Table 4.6 Atom Radii and Effective Ionic Radii of Elements         | 4.30        |
| <b>4.5.2</b> | <b>Ionic Radii</b>                                                 | <b>4.34</b> |
| <b>4.5.3</b> | <b>Covalent Radii</b>                                              | <b>4.35</b> |
|              | Table 4.7 Covalent Radii for Atoms                                 | 4.35        |
|              | Table 4.8 Octahedral Covalent Radii for CN = 6                     | 4.36        |
|              | Table 4.9 Bond Lengths between Carbon and Other Elements           | 4.36        |
|              | Table 4.10 Bond Lengths between Elements Other than Carbon         | 4.39        |
|              | Table 4.11 Bond Dissociation Energies                              | 4.41        |
| <b>4.6</b>   | <b>BOND AND GROUP DIPOLE MOMENTS</b>                               | <b>4.53</b> |
|              | Table 4.12 Bond Dipole Moments                                     | 4.53        |
|              | Table 4.13 Group Dipole Moments                                    | 4.54        |
| <b>4.7</b>   | <b>MOLECULAR GEOMETRY</b>                                          | <b>4.56</b> |
|              | Table 4.14 Spatial Orientation of Common Hybrid Bonds              | 4.56        |
|              | Figure 4.1 Crystal Lattice Types                                   | 4.57        |
|              | Table 4.15 Crystal Structure                                       | 4.58        |
| <b>4.8</b>   | <b>NUCLIDES</b>                                                    | <b>4.58</b> |
|              | Table 4.16 Table of Nuclides                                       | 4.58        |
| <b>4.9</b>   | <b>WORK FUNCTION</b>                                               | <b>4.80</b> |
|              | Table 4.17 Work Functions of the Elements                          | 4.80        |
| <b>4.10</b>  | <b>RELATIVE ABUNDANCES OF NATURALLY OCCURRING ISOTOPES</b>         | <b>4.81</b> |
|              | Table 4.18 Relative Abundances of Naturally Occurring Isotopes     | 4.81        |

---

### 4.1 ELEMENTS

---

The electronic configuration for an element's ground state (Table 4.1) is a shorthand representation giving the number of electrons (superscript) found in each of the allowed sublevels (*s*, *p*, *d*, *f*) above a noble gas core (indicated by brackets). In addition, values for the thermal conductivity, the electrical resistance, and the coefficient of linear thermal expansion are included.

**TABLE 4.1** Electronic Configuration and Properties of the Elements

| Name               | Symbol | Atomic number | Electronic configuration         | Thermal conductivity, $\text{W} \cdot (\text{m} \cdot \text{K})^{-1}$ at 25°C | Electrical resistivity, $\mu\Omega \cdot \text{cm}$ at 20°C | Coefficient of linear thermal expansion (25°C), $\text{m} \cdot \text{m}^{-1} (\times 10^6)$ |
|--------------------|--------|---------------|----------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------|----------------------------------------------------------------------------------------------|
| Actinium           | Ac     | 89            | [Rn] $6d^2 7s$                   | 12                                                                            |                                                             |                                                                                              |
| Aluminum           | Al     | 13            | [Ne] $3s^2 3p$                   | 237                                                                           | 2.6548                                                      | 23.1                                                                                         |
| Americium          | Am     | 95            | [Rn] $5f^7 7s^2$                 | 10                                                                            |                                                             |                                                                                              |
| Antimony (stibium) | Sb     | 51            | [Kr] $4d^{10} 5s^2 5p^3$         | 24.4                                                                          | 41.7                                                        | 11.0                                                                                         |
| Argon              | Ar     | 18            | [Ne] $3s^2 3p^6$                 | 0.017 72                                                                      |                                                             |                                                                                              |
| Arsenic            | As     | 33            | [Ar] $3d^{10} 4s^2 4p^3$         | 50.2                                                                          | 33.3                                                        |                                                                                              |
| Astatine           | At     | 85            | [Xe] $4f^{14} 5d^{10} 6s^2 6p^5$ | 1.7                                                                           |                                                             |                                                                                              |
| Barium             | Ba     | 56            | [Xe] $6s^2$                      | 18.4                                                                          | 33.2                                                        | 20.6                                                                                         |
| Berkelium          | Bk     | 97            | [Rn] $5f^8 6d 7s^2$              | 10                                                                            |                                                             |                                                                                              |
| Beryllium          | Be     | 4             | [He] $2s^2$                      | 200                                                                           | 3.56                                                        | 11.3                                                                                         |
| Bismuth            | Bi     | 83            | [Xe] $4f^{14} 5d^{10} 6s^2 6p^3$ | 7.97                                                                          | 129                                                         | 13.4                                                                                         |
| Boron              | B      | 5             | [He] $2s^2 2p$                   | 27.4                                                                          | $1.5 \times 10^{12}$                                        | 5–7                                                                                          |
| Bromine            | Br     | 35            | [Ar] $3d^{10} 4s^2 4p^5$         | 0.122                                                                         | $7.8 \times 10^{18}$                                        |                                                                                              |
| Cadmium            | Cd     | 48            | [Kr] $4d^{10} 5s^2$              | 96.6                                                                          | 7.27 (22°C)                                                 | 30.8                                                                                         |
| Calcium            | Ca     | 20            | [Ar] $4s^2$                      | 201                                                                           | 3.36                                                        | 22.3                                                                                         |
| Californium        | Cf     | 98            | [Rn] $5f^{10} 7s^2$              |                                                                               |                                                             |                                                                                              |
| Carbon             | C      | 6             | [He] $2s^2 2p^2$                 |                                                                               |                                                             |                                                                                              |
| (amorphous)        |        |               |                                  | 1.59                                                                          |                                                             |                                                                                              |
| (diamond)          |        |               |                                  | 900–2320                                                                      | 0.8                                                         |                                                                                              |
| (graphite)         |        |               |                                  | 119–165                                                                       | 1375                                                        |                                                                                              |
| Cerium             | Ce     | 58            | [Xe] $4f 5d 6s^2$                | 11.3                                                                          | 82.8 ( $\beta$ , hex)                                       | 6.3                                                                                          |
| Cesium             | Cs     | 55            | [Xe] $6s$                        | 35.9                                                                          | 20.5                                                        |                                                                                              |
| Chlorine           | Cl     | 17            | [Ne] $3s^2 3p^5$                 | 0.0089                                                                        | $>10^9$                                                     |                                                                                              |
| Chromium           | Cr     | 24            | [Ar] $3d^5 4s$                   | 93.9                                                                          | 12.5                                                        | 4.9                                                                                          |
| Cobalt             | Co     | 27            | [Ar] $3d^7 4s^2$                 | 100                                                                           | 6.24                                                        | 13.0                                                                                         |
| Copper (cuprum)    | Cu     | 29            | [Ar] $3d^{10} 4s$                | 401                                                                           | 1.678                                                       | 16.5                                                                                         |
| Curium             | Cm     | 96            | [Rn] $5f^7 6d 7s^2$              |                                                                               |                                                             |                                                                                              |
| Dysprosium         | Dy     | 66            | [Xe] $4f^{10} 6s^2$              | 10.7                                                                          | 92.6                                                        | 9.9                                                                                          |
| Einsteinium        | Es     | 99            | [Rn] $5f^{11} 7s^2$              |                                                                               |                                                             |                                                                                              |
| Erbium             | Er     | 68            | [Xe] $4f^{14} 6s^2$              | 14.5                                                                          | 86.0                                                        | 12.2                                                                                         |
| Europium           | Eu     | 63            | [Xe] $4f^7 6s^2$                 | 13.9                                                                          | 90.0                                                        | 35.0                                                                                         |

|                       |    |     |                                  |                            |                            |             |
|-----------------------|----|-----|----------------------------------|----------------------------|----------------------------|-------------|
| Fermium               | Fm | 100 | [Rn] $5f^{12} 7s^2$              |                            |                            |             |
| Fluorine              | F  | 9   | [He] $2s^2 2p^5$                 | 0.0277                     |                            |             |
| Francium              | Fr | 87  | [Rn] $7s$                        |                            |                            |             |
| Gadolinium            | Gd | 64  | [Xe] $4f^7 5d 6s^2$              | 10.5                       | 131                        | 9.4 (100°C) |
| Gallium               | Ga | 31  | [Ar] $3d^{10} 4s^2 4p$           | 29.4(lq) 40.6(c)           | 25.795 (30°C)              | 120         |
| Germanium             | Ge | 32  | [Ar] $3d^{10} 4s^2 4p^2$         | 60.2                       | 53 000                     | 6.0         |
| Gold (aurum)          | Au | 79  | [Xe] $4f^{14} 5d^{10} 6s$        | 318                        | 2.214                      | 14.2        |
| Hafnium               | Hf | 72  | [Xe] $4f^{14} 5d^2 6s^2$         | 23.0                       | 33.1                       | 5.9         |
| Helium                | He | 2   | $1s^2$                           | 0.1513                     |                            |             |
| Holmium               | Ho | 67  | [Xe] $4f^{11} 6s^2$              | 16.2                       | 81.4                       | 11.2        |
| Hydrogen              | H  | 1   | $1s$                             | 0.1805                     |                            |             |
| Indium                | In | 49  | [Kr] $4d^{10} 5s^2 5p$           | 81.8                       | 8.37                       | 32.1        |
| Iodine                | I  | 53  | [Kr] $4d^{10} 5s^2 5p^5$         | 449                        | $1.3 \times 10^{15}$ (0°C) |             |
| Iridium               | Ir | 77  | [Xe] $4f^{14} 5d^7 6s^2$         | 147                        | 4.71                       | 6.4         |
| Iron (ferrum)         | Fe | 26  | [Ar] $3d^6 4s^2$                 | 80.4                       | 9.61                       | 11.8        |
| Krypton               | Kr | 36  | [Ar] $3d^{10} 4s^2 4p^6$         | 9.43                       |                            |             |
| Lanthanum             | La | 57  | [Xe] $5d 6s^2$                   | 13.4                       | 61.5                       | 12.1        |
| Lawrencium            | Lr | 103 | [Rn] $4f^{14} 6d 7s^2$           |                            |                            |             |
| Lead (plumbum)        | Pb | 82  | [Xe] $4f^{14} 5d^{10} 6s^2 6p^2$ | 35.3                       | 20.8                       | 28.9        |
| Lithium               | Li | 3   | $1s^2 2s$                        | 84.8                       | 9.28                       | 46          |
| Lutetium              | Lu | 71  | [Xe] $4f^{14} 5d 6s^2$           | 16.4                       | 58.2                       | 9.9         |
| Magnesium             | Mg | 12  | [Ne] $3s^2$                      | 156                        | 4.39                       | 24.8        |
| Manganese             | Mn | 25  | [Ar] $3d^5 4s^2$                 | 7.81                       | 144                        | 21.7        |
| Mendelevium           | Md | 101 | [Rn] $5f^{13} 7s^2$              |                            |                            |             |
| Mercury (hydrargyrum) | Hg | 80  | [Xe] $4f^{14} 5d^{10} 6s^2$      | 8.30                       | 95.8(lq); 21(c)            |             |
| Molybdenum            | Mo | 42  | [Kr] $4d^5 5s$                   | 138                        | 5.34                       | 4.8         |
| Neodymium             | Nd | 60  | [Xe] $4f^4 6s^2$                 | 16.5                       | 64.3                       | 9.6         |
| Neon                  | Ne | 10  | $1s^2 2s^2 2p^6$                 | 0.0491                     |                            |             |
| Neptunium             | Np | 93  | [Rn] $5f^4 6d 7s^2$              | 6.3                        | 122.0 (22°C)               |             |
| Nickel                | Ni | 28  | [Ar] $3d^8 4s^2$                 | 90.9                       | 6.93                       | 13.4        |
| Niobium               | Nb | 41  | [Kr] $4d^4 5s$                   | 53.7                       | 15.2 (0°C)                 | 7.3         |
| Nitrogen              | N  | 7   | $1s^2 2s^2 2p^3$                 | 0.025 83                   |                            |             |
| Nobelium              | No | 102 | [Rn] $5f^{14} 7s^2$              |                            |                            |             |
| Osmium                | Os | 76  | [Xe] $4f^{14} 5d^6 6s^2$         | 87.6                       | 8.12 (0°C)                 | 5.1         |
| Oxygen                | O  | 8   | $1s^2 2s^2 2p^4$                 | 0.026 58 (g)<br>0.149 (lq) |                            |             |
| Palladium             | Pd | 46  | [Kr] $4d^{10}$                   | 71.8                       | 10.54                      | 11.8        |

**TABLE 4.1** Electronic Configuration and Properties of the Elements (*Continued*)

| Name                 | Symbol | Atomic number | Electronic configuration                                               | Thermal conductivity, $W \cdot (m \cdot K)^{-1}$ at 25°C | Electrical resistivity, $\mu\Omega \cdot cm$ at 20°C | Coefficient of linear thermal expansion (25°C), $m \cdot m^{-1} (\times 10^6)$ |
|----------------------|--------|---------------|------------------------------------------------------------------------|----------------------------------------------------------|------------------------------------------------------|--------------------------------------------------------------------------------|
| Phosphorus (white)   | P      | 15            | [Ne] 3s <sup>2</sup> 3p <sup>3</sup>                                   | 0.236 17                                                 | 10                                                   |                                                                                |
| Platinum             | Pt     | 78            | [Xe] 4f <sup>14</sup> 5d <sup>9</sup> 6s                               | 71.6                                                     | 10.6                                                 | 8.8                                                                            |
| Plutonium            | Pu     | 94            | [Rn] 5f <sup>6</sup> 7s <sup>2</sup>                                   | 6.74                                                     | 146.0 (0°C)                                          | 46.7                                                                           |
| Polonium             | Po     | 84            | [Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>4</sup> | 0.2                                                      | 40.0 (0°C) alpha                                     |                                                                                |
| Potassium (kalium)   | K      | 19            | [Ar] 4s                                                                | 102.5                                                    | 7.2                                                  |                                                                                |
| Praseodymium         | Pr     | 59            | [Xe] 4f <sup>3</sup> 6s <sup>2</sup>                                   | 12.5                                                     | 70.0                                                 | 6.7                                                                            |
| Promethium           | Pm     | 61            | [Xe] 4f <sup>5</sup> 6s <sup>2</sup>                                   | 17.9                                                     | 64.0 (25°C)                                          | est [11.]                                                                      |
| Protactinium         | Pa     | 91            | [Rn] 5f <sup>2</sup> 6d 7s <sup>2</sup>                                | 47                                                       | 19.1 (22°C)                                          |                                                                                |
| Radium               | Ra     | 88            | [Rn] 7s <sup>2</sup>                                                   | 18.6                                                     | 100                                                  |                                                                                |
| Radon                | Rn     | 86            | [Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>6</sup> | 0.003 61                                                 |                                                      |                                                                                |
| Rhenium              | Re     | 75            | [Xe] 5f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup>                  | 48.0                                                     | 19.3                                                 | 6.2                                                                            |
| Rhodium              | Rh     | 45            | [Kr] 4d <sup>8</sup> 5s                                                | 150                                                      | 4.33 (0°C)                                           | 8.2                                                                            |
| Rubidium             | Rb     | 37            | [Kr] 5s                                                                | 58.2                                                     | 12.8                                                 |                                                                                |
| Ruthenium            | Ru     | 44            | [Kr] 4d <sup>7</sup> 5s                                                | 117                                                      | 7.1 (0°C)                                            | 6.4                                                                            |
| Samarium             | Sm     | 62            | [Xe] 4f <sup>6</sup> 6s <sup>2</sup>                                   | 13.3                                                     | 94.0                                                 | 12.7                                                                           |
| Scandium             | Sc     | 21            | [Ar] 3d 4s <sup>2</sup>                                                | 15.8                                                     | 56.2                                                 | 10.2                                                                           |
| Selenium (amorphous) | Se     | 34            | [Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup>                  | 0.519                                                    | 1.2 (0°C)                                            | 37                                                                             |
| Silicon              | Si     | 14            | [Ne] 3s <sup>2</sup> 3p <sup>2</sup>                                   | 149                                                      | 10 <sup>5</sup>                                      |                                                                                |

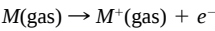
|                       |    |    |                                                           |           |                        |      |
|-----------------------|----|----|-----------------------------------------------------------|-----------|------------------------|------|
| Silver (argentum)     | Ag | 47 | [Kr] 4d <sup>10</sup> 5s                                  | 429       | 1.587                  | 18.9 |
| Sodium (natrium)      | Na | 11 | [Ne] 3s                                                   | 142       | 4.77                   | 71   |
| Strontium             | Sr | 38 | [Kr] 5s <sup>2</sup>                                      | 35.4      | 13.2                   | 22.5 |
| Sulfur (amorphous)    | S  | 16 | [Ne] 3s <sup>2</sup> 3p <sup>4</sup>                      | 0.205     | $2 \times 10^{23}$     |      |
| Tantalum              | Ta | 73 | [Xe] 4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup>     | 57.5      | 13.5                   | 6.3  |
| Technetium            | Tc | 43 | [Kr] 4d <sup>5</sup> 5s <sup>2</sup>                      | 50.6      | 22.6 (100°C)           |      |
| Tellurium             | Te | 52 | [Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup>     | 1.97–3.38 | $(5.8–33) \times 10^3$ |      |
| Terbium               | Tb | 65 | [Xe] 4f <sup>9</sup> 6s <sup>2</sup>                      | 11.1      | 115                    | 10.3 |
| Thallium              | Tl | 78 | [Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p | 46.1      | 18                     | 29.9 |
| Thorium               | Th | 90 | [Rn] 6d <sup>2</sup> 7s <sup>2</sup>                      | 54.0      | 15.4 (22°C)            | 11.1 |
| Thullium              | Tm | 69 | [Xe] 4f <sup>13</sup> 6s <sup>2</sup>                     | 16.9      | 67.6                   | 13.3 |
| Tin (stannum)         | Sn | 50 | [Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup>     | 66.8      | 11.5 (0°C)             | 22.0 |
| Titanium              | Ti | 22 | [Ar] 3d <sup>2</sup> 4s <sup>2</sup>                      | 21.9      | 42.0                   | 8.6  |
| Tungsten (wolframium) | W  | 74 | [Xe] 4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup>     | 173       | 5.28                   | 4.5  |
| Uranium               | U  | 92 | [Rn] 5f <sup>3</sup> 6d 7s <sup>2</sup>                   | 27.5      | 28.0 (0°C)             | 13.9 |
| Vanadium              | V  | 23 | [Ar] 3d <sup>3</sup> 4s <sup>2</sup>                      | 30.7      | 19.7                   | 8.4  |
| Xenon                 | Xe | 54 | [Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup>     | 0.005 65  |                        |      |
| Ytterbium             | Yb | 70 | [Xe] 4f <sup>14</sup> 6s <sup>2</sup>                     | 38.5      | 25                     | 26.3 |
| Yttrium               | Y  | 39 | [Kr] 4d 5s <sup>2</sup>                                   | 17.2      | 59.6                   | 10.6 |
| Zinc                  | Zn | 30 | [Ar] 3d <sup>10</sup> 4s <sup>2</sup>                     | 116       | 5.9                    | 30.2 |
| Zirconium             | Zr | 40 | [Kr] 4d <sup>2</sup> 5s <sup>2</sup>                      | 22.6      | 42.1                   | 5.7  |

**Source:** Ho, C. Y., Powell, R. W., and Liley, P. E., *J. Phys. Chem. Ref. Data* 3:Suppl. 1 (1974), (thermal conductivity); Ho, C. Y., et al., *J. Phys. Chem. Ref. Data*, 12:183 (1983); 13:1069, 1097, 1131 (1984), (electrical resistivity); Touloukian, Y. S., *Thermophysical Properties of Matter*, Vol. 12, *Thermal Expansion*, Plenum, New York, 1975.

4.2 IONIZATION ENERGY

TABLE 4.2 Ionization Energy of the Elements

The minimum amount of energy required to remove the least strongly bound electron from a gaseous atom (or ion) is called the ionization energy and is expressed in MJ · mol<sup>-1</sup>. Remember that 96.485 kJ = 1.000 eV = 23.0605 kcal. In Table 4.2 the successive stages of ionization are indicated by the heading of each column: I denotes first spectra arising from a neutral atom; viz.,



II, second spectra from singly ionized atoms, and so on for successive stages of ionization.

| At.<br>no. | Element | Spectrum (in MJ · mol <sup>-1</sup> ) |       |        |        |        |        |
|------------|---------|---------------------------------------|-------|--------|--------|--------|--------|
|            |         | I                                     | II    | III    | IV     | V      | VI     |
| 1          | H       | 1.312                                 |       |        |        |        |        |
| 2          | He      | 2.372                                 | 5.251 |        |        |        |        |
| 3          | Li      | 0.520                                 | 7.298 | 11.815 |        |        |        |
| 4          | Be      | 0.899                                 | 1.757 | 14.849 | 21.007 |        |        |
| 5          | B       | 0.801                                 | 2.427 | 3.660  | 25.027 | 32.828 |        |
| 6          | C       | 1.086                                 | 2.353 | 4.620  | 6.223  | 37.832 | 47.191 |
| 7          | N       | 1.402                                 | 2.856 | 4.578  | 7.475  | 9.445  | 53.268 |
| 8          | O       | 1.314                                 | 3.388 | 5.300  | 7.469  | 10.989 | 13.326 |
| 9          | F       | 1.681                                 | 3.374 | 6.147  | 8.408  | 11.022 | 15.164 |
| 10         | Ne      | 2.081                                 | 3.952 | 6.122  | 9.370  | 12.177 | 15.238 |
| 11         | Na      | 0.496                                 | 4.562 | 6.912  | 9.543  | 13.353 | 16.610 |
| 12         | Mg      | 0.738                                 | 1.451 | 7.733  | 10.540 | 13.629 | 17.994 |
| 13         | Al      | 0.578                                 | 1.817 | 2.745  | 11.577 | 14.831 | 18.377 |
| 14         | Si      | 0.786                                 | 1.577 | 3.231  | 4.355  | 16.091 | 19.784 |
| 15         | P       | 1.012                                 | 1.903 | 2.912  | 4.956  | 6.274  | 21.268 |
| 16         | S       | 1.000                                 | 2.251 | 3.361  | 4.564  | 7.004  | 8.495  |
| 17         | Cl      | 1.251                                 | 2.297 | 3.822  | 5.158  | 6.54   | 9.362  |
| 18         | Ar      | 1.521                                 | 2.666 | 3.931  | 5.771  | 7.238  | 8.787  |
| 19         | K       | 0.419                                 | 3.051 | 4.411  | 5.877  | 7.976  | 9.649  |
| 20         | Ca      | 0.590                                 | 1.145 | 4.912  | 6.474  | 8.144  | 10.496 |
| 21         | Sc      | 0.631                                 | 1.235 | 2.389  | 7.089  | 8.844  | 10.719 |
| 22         | Ti      | 0.658                                 | 1.310 | 2.652  | 4.175  | 9.573  | 11.516 |
| 23         | V       | 0.650                                 | 1.414 | 2.828  | 4.507  | 6.299  | 12.362 |
| 24         | Cr      | 0.653                                 | 1.592 | 2.987  | 4.743  | 6.70   | 8.738  |
| 25         | Mn      | 0.717                                 | 1.509 | 3.248  | 4.94   | 6.99   | 9.22   |
| 26         | Fe      | 0.759                                 | 1.561 | 2.957  | 5.63   | 7.24   | 9.56   |
| 27         | Co      | 0.758                                 | 1.646 | 3.232  | 4.95   | 7.67   | 9.84   |
| 28         | Ni      | 0.737                                 | 1.753 | 3.393  | 5.30   | 7.34   | 10.4   |
| 29         | Cu      | 0.745                                 | 1.958 | 3.555  | 5.536  | 7.70   | 9.9    |
| 30         | Zn      | 0.906                                 | 1.733 | 3.833  | 5.73   | 7.95   | 10.4   |
| 31         | Ga      | 0.579                                 | 1.979 | 2.963  | 6.2    |        |        |
| 32         | Ge      | 0.762                                 | 1.537 | 3.302  | 4.410  | 9.022  |        |
| 33         | As      | 0.947                                 | 1.798 | 2.735  | 4.837  | 6.043  | 12.31  |
| 34         | Se      | 0.941                                 | 2.045 | 2.974  | 4.143  | 6.99   | 7.883  |
| 35         | Br      | 1.140                                 | 2.10  | 3.47   | 4.56   | 5.76   | 8.55   |
| 36         | Kr      | 1.351                                 | 2.350 | 3.565  | 5.07   | 6.24   | 7.57   |
| 37         | Rb      | 0.403                                 | 2.632 | 3.9    | 5.08   | 6.85   | 8.14   |
| 38         | Sr      | 0.549                                 | 1.064 | 4.138  | 5.5    | 6.91   | 8.76   |
| 39         | Y       | 0.616                                 | 1.181 | 1.980  | 5.96   | 7.43   | 8.97   |
| 40         | Zr      | 0.660                                 | 1.267 | 2.218  | 3.313  | 7.75   |        |

**TABLE 4.2** Ionization Energy of the Elements (*Continued*)

| At.<br>no. | Element | Spectrum (in MJ · mol <sup>-1</sup> ) |       |       |       |       |       |
|------------|---------|---------------------------------------|-------|-------|-------|-------|-------|
|            |         | I                                     | II    | III   | IV    | V     | VI    |
| 41         | Nb      | 0.664                                 | 1.382 | 2.416 | 3.695 | 4.877 | 9.847 |
| 42         | Mo      | 0.685                                 | 1.558 | 2.621 | 4.477 | 5.91  | 6.641 |
| 43         | Tc      | 0.702                                 | 1.472 | 2.850 |       |       |       |
| 44         | Ru      | 0.711                                 | 1.617 | 2.747 |       |       |       |
| 45         | Rh      | 0.720                                 | 1.744 | 2.997 |       |       |       |
| 46         | Pd      | 0.805                                 | 1.875 | 3.177 |       |       |       |
| 47         | Ag      | 0.731                                 | 2.073 | 3.361 |       |       |       |
| 48         | Cd      | 0.868                                 | 1.631 | 3.616 |       |       |       |
| 49         | In      | 0.558                                 | 1.821 | 2.704 | 5.2   |       |       |
| 50         | Sn      | 0.709                                 | 1.412 | 2.943 | 3.930 | 6.974 |       |
| 51         | Sb      | 0.834                                 | 1.595 | 2.44  | 4.26  | 5.4   | 10.4  |
| 52         | Te      | 0.869                                 | 1.795 | 2.698 | 3.610 | 5.668 | 6.82  |
| 53         | I       | 1.008                                 | 1.846 | 3.2   |       |       |       |
| 54         | Xe      | 1.170                                 | 2.046 | 3.099 |       |       |       |
| 55         | Cs      | 0.376                                 | 2.234 |       |       |       |       |
| 56         | Ba      | 0.503                                 | 0.965 |       |       |       |       |
| 57         | La      | 0.538                                 | 1.067 | 1.850 | 4.820 | 5.94  |       |
| 58         | Ce      | 0.528                                 | 1.047 | 1.949 | 3.547 | 6.325 | 7.487 |
| 59         | Pr      | 0.523                                 | 1.018 | 2.086 | 3.761 | 5.551 |       |
| 60         | Nd      | 0.530                                 | 1.035 | 2.13  | 3.90  |       |       |
| 61         | Pm      | 0.535                                 | 1.052 | 2.15  | 3.97  |       |       |
| 62         | Sm      | 0.543                                 | 1.068 | 2.26  | 3.99  |       |       |
| 63         | Eu      | 0.547                                 | 1.085 | 2.40  | 4.12  |       |       |
| 64         | Gd      | 0.592                                 | 1.167 | 1.99  | 4.26  |       |       |
| 65         | Tb      | 0.564                                 | 1.112 | 2.114 | 3.839 |       |       |
| 66         | Dy      | 0.572                                 | 1.126 | 2.20  | 3.99  |       |       |
| 67         | Ho      | 0.581                                 | 1.139 | 2.204 | 4.10  |       |       |
| 68         | Er      | 0.589                                 | 1.151 | 2.194 | 4.13  |       |       |
| 69         | Tm      | 0.596                                 | 1.163 | 2.285 | 4.13  |       |       |
| 70         | Yb      | 0.603                                 | 1.174 | 2.417 | 4.203 |       |       |
| 71         | Lu      | 0.524                                 | 1.34  | 2.022 | 4.366 |       |       |
| 72         | Hf      | 0.68                                  | 1.44  | 2.25  | 3.216 |       |       |
| 73         | Ta      | 0.761                                 |       |       |       |       |       |
| 74         | W       | 0.770                                 |       |       |       |       |       |
| 75         | Re      | 0.760                                 |       |       |       |       |       |
| 76         | Os      | 0.84                                  |       |       |       |       |       |
| 77         | Ir      | 0.88                                  |       |       |       |       |       |
| 78         | Pt      | 0.87                                  | 1.791 |       |       |       |       |
| 79         | Au      | 0.890                                 | 1.98  |       |       |       |       |
| 80         | Hg      | 1.007                                 | 1.810 | 3.30  |       |       |       |
| 81         | Tl      | 0.589                                 | 1.971 | 2.878 |       |       |       |
| 82         | Pb      | 0.716                                 | 1.450 | 3.081 | 4.083 | 6.64  |       |
| 83         | Bi      | 0.703                                 | 1.610 | 2.466 | 4.371 | 5.40  | 8.52  |
| 84         | Po      | 0.812                                 |       |       |       |       |       |
| 85         | At      |                                       |       |       |       |       |       |
| 86         | Rn      | 1.037                                 |       |       |       |       |       |
| 87         | Fr      |                                       |       |       |       |       |       |
| 88         | Ra      | 0.509                                 | 0.979 |       |       |       |       |
| 89         | Ac      | 0.67                                  | 1.17  |       |       |       |       |
| 90         | Th      | 0.587                                 | 1.11  | 1.93  | 2.78  |       |       |
| 91         | Pa      | 0.568                                 |       |       |       |       |       |



**TABLE 4.2** Ionization Energy of the Elements (*Continued*)

| At.<br>no. | Element | Spectrum (in MJ · mol <sup>-1</sup> ) |    |     |    |   |    |
|------------|---------|---------------------------------------|----|-----|----|---|----|
|            |         | I                                     | II | III | IV | V | VI |
| 92         | U       | 0.598                                 |    |     |    |   |    |
| 93         | Np      | 0.605                                 |    |     |    |   |    |
| 94         | Pu      | 0.585                                 |    |     |    |   |    |
| 95         | Am      | 0.578                                 |    |     |    |   |    |
| 96         | Cm      | 0.581                                 |    |     |    |   |    |
| 97         | Bk      | 0.601                                 |    |     |    |   |    |
| 98         | Cf      | 0.608                                 |    |     |    |   |    |
| 99         | Es      | 0.619                                 |    |     |    |   |    |
| 100        | Fm      | 0.627                                 |    |     |    |   |    |
| 101        | Md      | 0.635                                 |    |     |    |   |    |
| 102        | No      | 0.642                                 |    |     |    |   |    |

**Source:** C. E. Moore, *National Standard Reference Data Series 34*, U.S. Government Printing Office, Washington, D.C., 1970; W. C. Martin, Zalubas, R., and Hagan, L., *J. Phys. Chem. Reference Data*, **3**:771 (1974) and National Standard Reference Data Series, National Bureau of Standards (U.S.), No. 60 (1978) for the Rare Earth Elements; and Cohen, E. R. and Taylor, B. N., *J. Phys. Chem. Reference Data*, **17**:1795 (1988).

**TABLE 4.3** Ionization Energy of Molecular and Radical Species

This table gives the first ionization potential in MJ · mol<sup>-1</sup> and in electron volts. Also listed is the enthalpy of formation of the ion at 25°C (298 K).

*Compounds containing carbon*

| Species            | Ionization energy         |                   | $\Delta_f H$ (ion)<br>in kJ · mol <sup>-1</sup> |
|--------------------|---------------------------|-------------------|-------------------------------------------------|
|                    | In MJ · mol <sup>-1</sup> | In electron volts |                                                 |
| Acenaphthene       | 0.741                     | 7.68              | 896                                             |
| Acenaphthylene     | 0.793                     | 8.22(4)           | 1053                                            |
| Acetaldehyde       | 0.98696(7)                | 10.2290(7)        | 821                                             |
| Acetamide          | 0.931(3)                  | 9.65(3)           | 693                                             |
| Acetic acid        | 1.029(2)                  | 10.66(2)          | 596                                             |
| Acetic anhydride   | 0.965                     | 10.0              | 398                                             |
| Acetone            | 0.9364                    | 9.705             | 719                                             |
| Acetonitrile       | 1.1766(5)                 | 12.194(5)         | 1252                                            |
| Acetophenone       | 0.896(3)                  | 9.29(3)           | 810                                             |
| Acetyl chloride    | 1.047(5)                  | 10.85(5)          | 804                                             |
| Acetyl fluoride    | 1.111(2)                  | 11.51(2)          | 667                                             |
| Acetylene          | 1.1000(2)                 | 11.400(2)         | 1328                                            |
| Allene             | 0.935(1)                  | 9.69(1)           | 1126                                            |
| Allyl alcohol      | 0.933(5)                  | 9.67(5)           | 808                                             |
| Allylamine         | 0.845                     | 8.76              | 891                                             |
| 3-Amino-1-propanol | 0.87                      | 9.0               | 651                                             |
| Aniline            | 0.7449(2)                 | 7.720(2)          | 832                                             |
| Anthracene         | 0.719(3)                  | 7.45(3)           | 949                                             |
| Azoxybenzene       | 0.78                      | 8.1               | 1123                                            |
| Azulene            | 0.715(2)                  | 7.41(2)           | 1004                                            |
| Benzaldehyde       | 0.916(2)                  | 9.49(2)           | 878                                             |
| Benzamide          | 0.912                     | 9.45              | 811                                             |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                     | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|-----------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                             | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Benzene                     | 0.89212(2)                           | 9.2459(2)         | 975                                                        |
| Benzenethiol                | 0.801(2)                             | 8.30(2)           | 913                                                        |
| Benzoic acid                | 0.914                                | 9.47              | 620                                                        |
| Benzonitrile                | 0.928                                | 9.62              | 1146                                                       |
| Benzophenone                | 0.873(5)                             | 9.05(5)           | 923                                                        |
| <i>p</i> -Benzoquinone      | 0.969(2)                             | 10.04(18)         | 847                                                        |
| Benzoyl chloride            | 0.920                                | 9.54              | 816                                                        |
| Benzyl alcohol              | 0.82                                 | 8.5               | 720                                                        |
| Benzylamine                 | 0.834(5)                             | 8.64(5)           | 917                                                        |
| Biphenyl                    | 0.767(2)                             | 7.95(2)           | 950                                                        |
| Bromoacetylene              | 0.995(2)                             | 10.31(2)          | 1242                                                       |
| Bromobenzene                | 0.866(2)                             | 8.98(2)           | 971                                                        |
| Bromochlorodifluoromethane  | 1.141                                | 11.83             | 702                                                        |
| Bromochloromethane          | 1.039(1)                             | 10.77(1)          | 1085                                                       |
| Bromodichloromethane        | 1.02                                 | 10.6              | 973                                                        |
| Bromoethane                 | 0.992                                | 10.28             | 930                                                        |
| Bromoethylene               | 0.946(2)                             | 9.80(2)           | 1025                                                       |
| Bromomethane                | 1.0171(3)                            | 10.541(3)         | 979                                                        |
| 1-Bromonaphthalene          | 0.781                                | 8.09              | 956                                                        |
| Bromopentafluorobenzene     | 0.923(2)                             | 9.57(2)           | 212                                                        |
| 1-Bromopropane              | 0.982(1)                             | 10.18(1)          | 898                                                        |
| 2-Bromopropane              | 0.972(1)                             | 10.07(1)          | 874                                                        |
| 3-Bromopropene              | 0.972(1)                             | 10.07(1)          | 1018                                                       |
| <i>p</i> -Bromotoluene      | 0.837(1)                             | 8.67(1)           | 908                                                        |
| Bromotrichloromethane       | 1.02                                 | 10.6              | 980                                                        |
| Bromotrifluoromethane       | 1.10                                 | 11.4              | 451                                                        |
| 1,2-Butadiene               | 0.871                                | 9.03              | 1034                                                       |
| 1,3-Butadiene               | 0.8750                               | 9.069             | 985                                                        |
| Butanal                     | 0.949(2)                             | 9.84(2)           | 742                                                        |
| Butanenitrile               | 1.08                                 | 11.2              | 1110                                                       |
| 2-Butanone                  | 0.918(4)                             | 9.51(4)           | 677                                                        |
| <i>trans</i> -2-Butenal     | 0.939(1)                             | 9.73(1)           | 835                                                        |
| 1-Butene                    | 0.924(2)                             | 9.58(2)           | 924                                                        |
| <i>cis</i> -2-Butene        | 0.8788(8)                            | 9.108(8)          | 871                                                        |
| <i>trans</i> -2-Butene      | 0.8780(8)                            | 9.100(8)          | 866                                                        |
| 1-Buten-3-yne               | 0.924(2)                             | 9.58(2)           | 1230                                                       |
| Butyl acetate               | 0.965                                | 10.0              | 479                                                        |
| <i>sec</i> -Butyl acetate   | 0.955                                | 9.90              | 453                                                        |
| Butyl ethyl ether           | 0.903                                | 9.36              | 610                                                        |
| Butylbenzene                | 0.838(1)                             | 8.69(1)           | 826                                                        |
| <i>sec</i> -Butylbenzene    | 0.837(1)                             | 8.68(1)           | 820                                                        |
| <i>tert</i> -Butylbenzene   | 0.834(2)                             | 8.64(2)           | 812                                                        |
| Butylcyclohexane            | 0.908                                | 9.41              | 695                                                        |
| Butylcyclopentane           | 0.960(3)                             | 9.95(3)           | 793                                                        |
| <i>p-tert</i> -Butylphenol  | 0.75                                 | 7.8               | 552                                                        |
| <i>p-tert</i> -Butyltoluene | 0.799                                | 8.28              | 745                                                        |
| 1-Butyne                    | 0.9821(5)                            | 10.178(5)         | 1147                                                       |
| 2-Butyne                    | 0.9226(5)                            | 9.562(5)          | 1068                                                       |
| Camphor                     | 0.845(3)                             | 8.76(3)           | 577                                                        |
| Caprolactam                 | 0.875(2)                             | 9.07(2)           | 629                                                        |
| Carbazole                   | 0.730(3)                             | 7.57(3)           | 961                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                          | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|--------------------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                                  | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Carbon                                           | 1.0865                               | 11.260            | 1803                                                       |
| Carbon ( $\text{C}_2$ )                          | 1.188                                | 12.31             | 2000                                                       |
| Carbon dioxide                                   | 1.3289(2)                            | 13.773(2)         | 935                                                        |
| Carbon monoxide                                  | 1.35217                              | 14.0139           | 1242                                                       |
| Carbon oxyselenide                               | 1.000(1)                             | 10.36(1)          | 929                                                        |
| Carbon oxysulfide                                | 1.07812(15)                          | 11.1736(15)       | 936                                                        |
| Carbon sulfide                                   | 0.97149(19)                          | 10.0685(20)       | 1089                                                       |
| Carbon sulfide (CS)                              | 1.093(1)                             | 11.33(1)          | 1368                                                       |
| Carbonyl fluoride                                | 1.257                                | 13.03             | 617                                                        |
| Carbonyltrihydroboron ( $\text{BH}_3\text{CO}$ ) | 1.075(2)                             | 11.14(2)          | 962                                                        |
| Chloroacetaldehyde                               | 1.011(3)                             | 10.48(3)          | 815                                                        |
| Chloroacetic acid                                | 0.984                                | 10.2              | 597                                                        |
| Chloroacetyl chloride                            | 1.06                                 | 11.0              | 815                                                        |
| Chloroacetylene                                  | 1.021(2)                             | 10.58(2)          | 1276                                                       |
| <i>m</i> -Chloroaniline                          | 0.781(10)                            | 8.09(10)          | 835                                                        |
| <i>o</i> -Chloroaniline                          | 0.820                                | 8.50              | 883                                                        |
| <i>p</i> -Chloroaniline                          | 0.789                                | 8.18              | 844                                                        |
| Chlorobenzene                                    | 0.874(2)                             | 9.06(2)           | 929                                                        |
| Chlorodibromomethane                             | 0.1022(1)                            | 10.59(1)          | 1030                                                       |
| 1-Chloro-1,1-difluoroethane                      | 1.156(1)                             | 11.98(1)          | 626                                                        |
| 1-Chloro-2,2-difluoroethylene                    | 0.946(4)                             | 9.80(4)           | 628                                                        |
| Chlorodifluoromethane                            | 1.18                                 | 12.2              | 693                                                        |
| Chloroethane                                     | 1.058(2)                             | 10.97(2)          | 946                                                        |
| 2-Chloroethanol                                  | 1.015                                | 10.52             | 756                                                        |
| Chloroethylene                                   | 0.964(2)                             | 9.99(2)           | 985                                                        |
| Chlorofluoromethane                              | 1.130(1)                             | 11.71(1)          | 870                                                        |
| Chloromethane                                    | 1.083(1)                             | 11.22(1)          | 1001                                                       |
| Chloromethylene                                  | 0.949                                | 9.84              | 1247                                                       |
| Chloromethylidene ( $\text{CCl}$ )               | 0.86(2)                              | 8.9(2)            | 1244                                                       |
| 1-Chloronaphthalene                              | 0.784                                | 8.13              | 906                                                        |
| <i>m</i> -Chloronitrobenzene                     | 0.957(10)                            | 9.92(10)          | 995                                                        |
| <i>p</i> -Chloronitrobenzene                     | 0.961(10)                            | 9.96(10)          | 999                                                        |
| Chloropentafluorobenzene                         | 0.938(2)                             | 9.72(2)           | 126                                                        |
| Chloropentafluoroethane                          | 1.22                                 | 12.6              | 99                                                         |
| <i>m</i> -Chlorophenol                           | 0.835                                | 8.65              | 680                                                        |
| <i>p</i> -Chlorophenol                           | 0.834                                | 8.69              | 692                                                        |
| 1-Chloropropane                                  | 1.044(3)                             | 10.82(3)          | 912                                                        |
| 2-Chloropropane                                  | 1.040(2)                             | 10.78(2)          | 895                                                        |
| 3-Chloropropene                                  | 0.96                                 | 9.9               | 950                                                        |
| <i>m</i> -Chlorotoluene                          | 0.852(2)                             | 8.83(2)           | 869                                                        |
| <i>o</i> -Chlorotoluene                          | 0.852(2)                             | 8.83(2)           | 869                                                        |
| <i>p</i> -Chlorotoluene                          | 0.838(2)                             | 8.69(2)           | 855                                                        |
| Chlorotrifluoroethylene                          | 0.947                                | 9.81(3)           | 373                                                        |
| Chlorotrifluoromethane                           | 1.195                                | 12.39             | 485                                                        |
| Chrysene                                         | 0.732                                | 7.59(2)           | 1016                                                       |
| Coronene                                         | 0.703                                | 7.29              | 1026                                                       |
| <i>m</i> -Cresol                                 | 0.800                                | 8.29              | 668                                                        |
| <i>o</i> -Cresol                                 | 0.785                                | 8.14              | 660                                                        |
| <i>p</i> -Cresol                                 | 0.784                                | 8.13              | 659                                                        |
| <i>cis</i> -Crotonic acid                        | 0.973                                | 10.08             | 625                                                        |
| <i>trans</i> -Crotonic acid                      | 0.96                                 | 9.9               | 604                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                            | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                    | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Cumene                             | 0.842                                | 8.73(1)           | 847                                                        |
| Cyanamide                          | 1.00                                 | 10.4              | 1137                                                       |
| Cyanate (NCO)                      | 1.135(1)                             | 11.76(1)          | 1290                                                       |
| Cyanide (CN)                       | 1.360                                | 14.09             | 1795                                                       |
| Cyanoacetylene                     | 1.123(1)                             | 11.64(1)          | 1475                                                       |
| Cyanogen                           | 1.290(1)                             | 13.37(1)          | 1597                                                       |
| Cyanogen chloride                  | 1.191(1)                             | 12.34(1)          | 1329                                                       |
| Cyanogen fluoride                  | 1.285(1)                             | 13.32(1)          | 1323                                                       |
| Cyclobutane                        | 0.957(5)                             | 9.92(5)           | 986                                                        |
| Cyclobutanone                      | 0.9025                               | 9.354             | 815                                                        |
| Cyclobutene                        | 0.910                                | 9.43              | 1067                                                       |
| Cycloheptane                       | 0.962                                | 9.97              | 844                                                        |
| Cyclohexane                        | 0.951(3)                             | 9.86(3)           | 828                                                        |
| Cyclohexanol                       | 0.941                                | 9.75              | 651                                                        |
| Cyclohexanone                      | 0.882(1)                             | 9.14(1)           | 656                                                        |
| Cyclohexene                        | 0.8631(10)                           | 8.945(10)         | 859                                                        |
| Cyclohexylamine                    | 0.832(23)                            | 8.62(24)          | 727                                                        |
| Cyclohexylcyclohexane              | 0.908                                | 9.41              | 690                                                        |
| Cyclooctane                        | 0.942                                | 9.76              | 817                                                        |
| Cyclopropane                       | 0.951                                | 9.86              | 1005                                                       |
| Cyclopropanecarbonitrile           | 0.989                                | 10.25             | 1173                                                       |
| Cyclopropanone                     | 0.88(1)                              | 9.1(1)            | 895                                                        |
| Cyclopropene                       | 0.930                                | 9.67(1)           | 1209                                                       |
| Cyclopropylamine                   | 0.84                                 | 8.7               | 916                                                        |
| Cyclopropylbenzene                 | 0.806                                | 8.35              | 956                                                        |
| <i>cis</i> -Decahydronaphthalene   | 0.893                                | 9.26              | 724                                                        |
| <i>trans</i> -Decahydronaphthalene | 0.892                                | 9.24              | 710                                                        |
| Decane                             | 0.931                                | 9.65              | 682                                                        |
| 1-Decene                           | 0.909(1)                             | 9.42(1)           | 786                                                        |
| Diazomethane                       | 0.8683(1)                            | 8.999(1)          | 1098                                                       |
| 1,4-Dibromobutane                  | 0.979                                | 10.15             | 879                                                        |
| 1,2-Dibromoethane                  | 1.001                                | 10.37             | 963                                                        |
| Dibromofluoromethane               | 1.069(3)                             | 11.07(3)          | 687                                                        |
| Dibromomethane                     | 1.013(2)                             | 10.50(2)          | 1013                                                       |
| 1,2-Dibromopropane                 | 0.975                                | 10.1              | 903                                                        |
| 1,3-Dibromopropane                 | 0.990                                | 10.26             | 919                                                        |
| 1,2-Dibromotetrafluoroethane       | 1.07                                 | 11.1              | 280                                                        |
| Dibutyl ether                      | 0.910                                | 9.43              | 575                                                        |
| Di- <i>sec</i> -butyl ether        | 0.879                                | 9.11              | 511                                                        |
| Di- <i>tert</i> -butyl ether       | 0.850                                | 8.81              | 486                                                        |
| Dibutyl sulfide                    | 0.79                                 | 8.2               | 624                                                        |
| Di- <i>tert</i> -butyl sulfide     | 0.77                                 | 8.0               | 583                                                        |
| Dibutylamine                       | 0.742(3)                             | 7.69(3)           | 586                                                        |
| Dichloroacetyl chloride            | 1.06                                 | 11.0              | 819                                                        |
| Dichloroacetylene                  | 0.974                                | 10.09             | 1183                                                       |
| <i>m</i> -Dichlorobenzene          | 0.879(1)                             | 9.11(1)           | 907                                                        |
| <i>o</i> -Dichlorobenzene          | 0.876(1)                             | 9.08(1)           | 909                                                        |
| <i>p</i> -Dichlorobenzene          | 0.856(1)                             | 8.89(1)           | 882                                                        |
| Dichlorodifluoromethane            | 1.134(4)                             | 11.75(4)          | 656                                                        |
| Dichlorodimethylsilane             | 1.03                                 | 10.7              | 576                                                        |
| 1,1-Dichloroethane                 | 1.067                                | 11.06             | 937                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                             | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|-------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                     | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| 1,2-Dichloroethane                  | 1.065                                | 11.04             | 931                                                        |
| 1,1-Dichloroethylene                | 0.945(4)                             | 9.79(4)           | 947                                                        |
| <i>cis</i> -1,2-Dichloroethylene    | 0.932(1)                             | 9.66(1)           | 936                                                        |
| <i>trans</i> -1,2-Dichloroethylene  | 0.931(2)                             | 9.65(2)           | 935                                                        |
| Dichlorofluoromethane               | 1.11                                 | 11.5              | 829                                                        |
| Dichloromethane                     | 1.092(1)                             | 11.32(1)          | 996                                                        |
| Dichloromethylene                   | 1.000                                | 10.36             | 1163                                                       |
| 1,2-Dichloropropane                 | 1.049(5)                             | 10.87(5)          | 886                                                        |
| 1,3-Dichloropropane                 | 1.047(5)                             | 10.85(5)          | 888                                                        |
| 1,2-Dichlorotetrafluoroethane       | 1.18                                 | 12.2              | 252                                                        |
| Dicyclopropyl ketone                | 0.88                                 | 9.1               | 1041                                                       |
| 1,1-Diethoxyethane                  | 0.944                                | 9.78              | 490                                                        |
| Diethyl oxalate                     | 0.95                                 | 9.8               | 205                                                        |
| <i>m</i> -Diethylbenzene            | 0.819(1)                             | 8.49(1)           | 798                                                        |
| <i>o</i> -Diethylbenzene            | 0.821                                | 8.51              | 804                                                        |
| <i>p</i> -Diethylbenzene            | 0.810                                | 8.40              | 790                                                        |
| Diethylene glycol dimethyl ether    | 0.96                                 | 9.8               | 448                                                        |
| <i>m</i> -Difluorobenzene           | 0.900(1)                             | 9.33(1)           | 591                                                        |
| <i>o</i> -Difluorobenzene           | 0.895(1)                             | 9.28(1)           | 602                                                        |
| <i>p</i> -Difluorobenzene           | 0.882(1)                             | 9.14(1)           | 575                                                        |
| 1,1-Difluoroethane                  | 1.145(3)                             | 11.87(3)          | 643                                                        |
| 1,1-Difluoroethylene                | 0.993(1)                             | 10.29(1)          | 650                                                        |
| <i>cis</i> -1,2-Difluoroethylene    | 0.987                                | 10.23             | 690                                                        |
| Difluoromethane                     | 1.226                                | 12.71             | 774                                                        |
| Difluoromethylene                   | 1.102(1)                             | 11.42(1)          | 897                                                        |
| 2,5-Dihydrothiophene                | 0.81                                 | 8.4               | 898                                                        |
| Diiodomethane                       | 0.913(2)                             | 9.46(2)           | 1030                                                       |
| Diisobutyl sulfide                  | 0.807(5)                             | 8.36(5)           | 627                                                        |
| Diisobutylamine                     | 0.754                                | 7.81              | 574                                                        |
| Diisopropyl ether                   | 0.888(5)                             | 9.20(5)           | 569                                                        |
| Diisopropyl sulfide                 | 0.833(5)                             | 8.63(5)           | 630                                                        |
| Diisopropylamine                    | 0.746(3)                             | 7.73(3)           | 602                                                        |
| Diketene                            | 0.93(2)                              | 9.6(2)            | 736                                                        |
| Dimethoxymethane                    | 0.92                                 | 9.5               | 569                                                        |
| Dimethyl disulfide                  | 0.71                                 | 7.4(3)            | 690                                                        |
| Dimethyl ether                      | 0.9673(23)                           | 10.025(25)        | 783                                                        |
| Dimethyl oxalate                    | 0.965                                | 10.0              | 287                                                        |
| <i>o</i> -Dimethyl phthalate        | 0.930(7)                             | 9.64(7)           | 277                                                        |
| Dimethyl sulfide                    | 0.838(1)                             | 8.69(1)           | 801                                                        |
| Dimethyl sulfoxide                  | 0.878                                | 9.01              | 718                                                        |
| Dimethylamine                       | 0.794(8)                             | 8.23(8)           | 776                                                        |
| <i>N,N</i> -Dimethylaniline         | 0.687(2)                             | 7.12(2)           | 787                                                        |
| 2,2-Dimethylbutane                  | 0.971                                | 10.06             | 787                                                        |
| 2,3-Dimethylbutane                  | 0.967                                | 10.02             | 791                                                        |
| 3,3-Dimethyl-2-butanone             | 0.879(2)                             | 9.11(2)           | 589                                                        |
| 2,3-Dimethyl-1-butene               | 0.875(1)                             | 9.07(1)           | 812                                                        |
| 2,3-Dimethyl-2-butene               | 0.798(1)                             | 8.27(1)           | 729                                                        |
| 3,3-Dimethyl-1-butyne               | 0.946(5)                             | 9.80(5)           | 1050                                                       |
| 1,1-Dimethylcyclohexane             | 0.909                                | 9.42              | 728                                                        |
| <i>cis</i> -1,2-Dimethylcyclohexane | <0.944                               | <9.78             | 772                                                        |
| <i>cis</i> -1,3-Dimethylcyclohexane | <0.963                               | <9.98             | 778                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                   | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|-------------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                           | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| <i>cis</i> -1,4-Dimethylcyclohexane       | <0.958                               | <9.93             | 782                                                        |
| <i>trans</i> -1,2-Dimethylcyclohexane     | 0.908                                | 9.41              | 728                                                        |
| <i>trans</i> -1,3-Dimethylcyclohexane     | 0.920                                | 9.53              | 743                                                        |
| <i>trans</i> -1,4-Dimethylcyclohexane     | 0.922                                | 9.56              | 738                                                        |
| <i>cis</i> -1,2-Dimethylcyclopentane      | 0.957(5)                             | 9.92(5)           | 828                                                        |
| <i>trans</i> -1,2-Dimethylcyclopentane    | 0.960(5)                             | 9.95(5)           | 823                                                        |
| <i>N,N</i> -Dimethylformamide             | 0.881(2)                             | 9.13(2)           | 689                                                        |
| 2,6-Dimethyl-4-heptanone                  | 0.872(3)                             | 9.04(3)           | 515                                                        |
| 1,1-Dimethylhydrazine                     | 0.702(4)                             | 7.28(4)           | 786                                                        |
| 2,4-Dimethyl-3-pentanone                  | 0.864(1)                             | 8.95(1)           | 552                                                        |
| 2,3-Dimethylpyridine                      | 0.854(2)                             | 8.85(2)           | 922                                                        |
| 2,4-Dimethylpyridine                      | 0.854(3)                             | 8.85(3)           | 918                                                        |
| 2,5-Dimethylpyridine                      | 0.849(5)                             | 8.80(5)           | 916                                                        |
| 2,6-Dimethylpyridine                      | 0.847(3)                             | 8.86(3)           | 913                                                        |
| 3,4-Dimethylpyridine                      | 0.883                                | 9.15              | 953                                                        |
| 3,5-Dimethylpyridine                      | 0.893                                | 9.25              | 965                                                        |
| <i>N,N</i> -Dimethyl- <i>o</i> -toluidine | 0.714(2)                             | 7.40(2)           | 814                                                        |
| 1,3-Dioxane                               | 0.95                                 | 9.8               | 607                                                        |
| 1,4-Dioxane                               | 0.887(1)                             | 9.19(1)           | 571                                                        |
| 1,3-Dioxolane                             | 0.96                                 | 9.9               | 658                                                        |
| Diphenyl ether                            | 0.781(3)                             | 8.09(3)           | 766                                                        |
| Diphenylacetylene                         | 0.762(2)                             | 7.90(2)           | 1164                                                       |
| Diphenylamine                             | 0.691(4)                             | 7.16(4)           | 908                                                        |
| 1,2-Diphenylethane                        | 0.84(1)                              | 8.7(1)            | 983                                                        |
| Diphenylmethane                           | 0.825(3)                             | 8.55(3)           | 963                                                        |
| Dipropyl ether                            | 0.894(5)                             | 9.27(5)           | 602                                                        |
| Dipropyl sulfide                          | 0.801(2)                             | 8.30(2)           | 676                                                        |
| Dipropylamine                             | 0.746(3)                             | 7.73(3)           | 641                                                        |
| Divinyl ether                             | 0.84                                 | 8.7               | 827                                                        |
| 5,7-Dodecadiyne                           | 0.837                                | 8.67              | 1079                                                       |
| Dodecafluorocyclohexane                   | 1.27                                 | 13.2              | −1095                                                      |
| Epichlorohydrin                           | 0.98                                 | 10.2              | 875                                                        |
| 1,2-Epoxybutane                           | 0.98                                 | 10.15             | 862                                                        |
| Ethane                                    | 1.112(1)                             | 11.52(1)          | 1027                                                       |
| 1,2-Ethanediamine                         | 0.83                                 | 8.6               | 812                                                        |
| Ethanethiol                               | 0.8959(5)                            | 9.285(5)          | 849                                                        |
| Ethanol                                   | 1.010(2)                             | 10.47(2)          | 776                                                        |
| Ethanolamine                              | 0.865                                | 8.96              | 664                                                        |
| Ethyl benzoate                            | 0.86                                 | 8.9               | 537                                                        |
| Ethyl formate                             | 1.024(1)                             | 10.61(1)          | 639                                                        |
| Ethyl methyl ether                        | 0.938                                | 9.72              | 722                                                        |
| Ethyl methyl sulfide                      | 0.824(10)                            | 8.54(10)          | 765                                                        |
| Ethyl pentyl ether                        | 9.16                                 | 9.49              | 602                                                        |
| Ethyl vinyl ether                         | 0.85                                 | 8.8               | 707                                                        |
| Ethylamine                                | 0.855(2)                             | 8.86(2)           | 808                                                        |
| <i>N</i> -Ethylaniline                    | 0.740                                | 7.67              | 794                                                        |
| Ethylbenzene                              | 0.846(1)                             | 8.77(1)           | 876                                                        |
| 2-Ethyl-1-butene                          | 0.874(2)                             | 9.06(2)           | 818                                                        |
| Ethylcyclohexane                          | 0.920                                | 9.54              | 748                                                        |
| Ethylcyclopentane                         | 0.976(2)                             | 10.12(2)          | 850                                                        |
| Ethylene                                  | 1.0382(4)                            | 10.507(4)         | 1066                                                       |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                               | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|---------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                       | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Ethylene glycol                       | 0.980                                | 10.16             | 593                                                        |
| Ethylene oxide                        | 1.0195(10)                           | 10.566(10)        | 967                                                        |
| Ethyleneimine                         | 0.89(1)                              | 9.2(1)            | 1014                                                       |
| <i>p</i> -Ethylphenol                 | 0.756                                | 7.84              | 613                                                        |
| Ethynyl ( $\text{HC}\equiv\text{C}$ ) | 1.13                                 | 11.7              | 1694                                                       |
| Fluoranthene                          | 0.768(4)                             | 7.95(4)           | 1057                                                       |
| Fluorene                              | 0.761(3)                             | 7.89(3)           | 950                                                        |
| Fluoroacetylene                       | 1.086                                | 11.26             | 1195                                                       |
| Fluorobenzene                         | 0.8877(5)                            | 9.200(5)          | 772                                                        |
| Fluoroethane                          | 1.12                                 | 11.6              | 856                                                        |
| Fluoroethylene                        | 1.0000(15)                           | 10.363(15)        | 861                                                        |
| Fluoromethane                         | 1.203(2)                             | 12.47(2)          | 956                                                        |
| Fluoromethylene                       | 1.012                                | 10.49             | 1121                                                       |
| Fluoromethylidene ( $\text{CF}$ )     | 0.879(1)                             | 9.11(1)           | 1134                                                       |
| <i>p</i> -Fluoronitrobenzene          | 0.955                                | 9.90              | 826                                                        |
| 1-Fluoropropane                       | 1.09                                 | 11.3              | 806                                                        |
| 2-Fluoropropane                       | 1.069(2)                             | 11.08(2)          | 776                                                        |
| 3-Fluoropropene                       | 0.975                                | 10.11             | 821                                                        |
| <i>m</i> -Fluorotoluene               | 0.860(1)                             | 8.91(1)           | 709                                                        |
| <i>o</i> -Fluorotoluene               | 0.860(1)                             | 8.91(1)           | 709                                                        |
| <i>p</i> -Fluorotoluene               | 0.848(1)                             | 8.79(1)           | 701                                                        |
| Formaldehyde                          | 1.0492(2)                            | 10.874(2)         | 940                                                        |
| Formamide                             | 0.980(6)                             | 10.16(6)          | 796                                                        |
| Formic acid                           | 1.093(1)                             | 11.33(1)          | 715                                                        |
| Fulminic acid ( $\text{HCNO}$ )       | 1.045                                | 10.83             | 1263                                                       |
| Fulvene                               | 0.807                                | 8.36              | 1031                                                       |
| Fumaric acid                          | 1.03                                 | 10.7              | 355                                                        |
| Furan                                 | 0.8571(3)                            | 8.883(3)          | 822                                                        |
| Glyoxal                               | 0.975                                | 10.1              | 763                                                        |
| 1-Heptanal                            | 0.931(2)                             | 9.65(2)           | 668                                                        |
| Heptane                               | 0.957(5)                             | 9.92(5)           | 770                                                        |
| 1-Heptanol                            | 0.949(3)                             | 9.84(3)           | 614                                                        |
| 2-Heptanol                            | 0.936(3)                             | 9.70(3)           | 580                                                        |
| 3-Heptanol                            | 0.934(3)                             | 9.68(3)           | 578                                                        |
| 4-Heptanol                            | 0.927(3)                             | 9.61(3)           | 572                                                        |
| 2-Heptanone                           | 0.897(1)                             | 9.30(1)           | 596                                                        |
| 1-Heptene                             | 0.911                                | 9.44              | 849                                                        |
| 2-Heptene                             | 0.853(2)                             | 8.84(2)           | 782                                                        |
| 3-Heptene                             | 0.861                                | 8.92              | 790                                                        |
| Hexachlorobenzene                     | 0.866                                | 8.98              | 822                                                        |
| Hexachloroethane                      | 1.07                                 | 11.1              | 920                                                        |
| 1,5-Hexadiene                         | 0.896(5)                             | 9.29(5)           | 980                                                        |
| Hexafluoroacetone                     | 1.104                                | 11.44             | − 294                                                      |
| Hexafluorobenzene                     | 0.9558                               | 9.906             | 10                                                         |
| Hexafluoroethane                      | 1.29                                 | 13.4              | − 50                                                       |
| Hexafluoropropene                     | 1.023(3)                             | 10.60(3)          | − 103                                                      |
| Hexamethylbenzene                     | 0.757                                | 7.85              | 670                                                        |
| 1-Hexanal                             | 0.933(5)                             | 9.67(5)           | 686                                                        |
| Hexane                                | 0.977                                | 10.13             | 810                                                        |
| Hexanoic acid                         | 0.976                                | 10.12             | 463                                                        |
| 1-Hexanol                             | 0.954(3)                             | 9.89(3)           | 639                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                       | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|-------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                               | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| 2-Hexanol                     | 0.946(3)                             | 9.80(3)           | 611                                                        |
| 3-Hexanol                     | 0.929(3)                             | 9.63(3)           | 599                                                        |
| 2-Hexanone                    | 0.902(2)                             | 9.35(2)           | 626                                                        |
| 3-Hexanone                    | 0.880(2)                             | 9.12(2)           | 600                                                        |
| 1-Hexene                      | 0.911(4)                             | 9.44(4)           | 869                                                        |
| <i>cis</i> -2-Hexene          | 0.865(1)                             | 8.97(1)           | 818                                                        |
| <i>trans</i> -2-Hexene        | 0.865(1)                             | 8.97(1)           | 814                                                        |
| Hexylamine                    | 0.833(5)                             | 8.63(5)           | 699                                                        |
| 1-Hexyne                      | 0.960                                | 9.95(5)           | 1081                                                       |
| Hydrogen cyanide (HCN)        | 1.312(1)                             | 13.60(1)          | 1447                                                       |
| Hydrogen isocyanide (HNC)     | 1.21(1)                              | 12.5(1)           | 1407                                                       |
| <i>p</i> -Hydroquinone        | 0.767(3)                             | 7.95(3)           | 504                                                        |
| Imidazole                     | 0.850(1)                             | 8.81(1)           | 997                                                        |
| Indane                        | 0.90                                 | 9.3               | 864                                                        |
| Indene                        | 0.785(1)                             | 8.14(1)           | 949                                                        |
| Iodobenzene                   | 0.8380                               | 8.685             | 1003                                                       |
| Iodoethane                    | 0.9018                               | 9.346             | 893                                                        |
| 1-Iodohexane                  | 0.8857                               | 9.179             | 794                                                        |
| Iodomethane                   | 0.9203                               | 9.538             | 936                                                        |
| 1-Iodopropane                 | 0.8943                               | 9.269             | 862                                                        |
| 2-Iodopropane                 | 0.8853                               | 9.175             | 844                                                        |
| Isobutylbenzene               | 0.838(1)                             | 8.68(1)           | 816                                                        |
| Isocyanic acid                | 1.120(3)                             | 11.61(3)          | 1016                                                       |
| Isophthalic acid              | 0.963(20)                            | 9.98(20)          | 268                                                        |
| Isopropylcyclohexane          | 0.900                                | 9.33              | 704                                                        |
| Isoquinoline                  | 0.8239(3)                            | 8.539(3)          | 1032                                                       |
| Isoxazole                     | 0.958(5)                             | 9.93(5)           | 1038                                                       |
| Ketene                        | 0.927(2)                             | 9.61(2)           | 880                                                        |
| Maleic anhydride              | 1.04                                 | 10.8              | 645                                                        |
| Mesityl oxide                 | 0.876(3)                             | 9.08(3)           | 692                                                        |
| Methacrylic acid              | 0.979                                | 10.15             | 611                                                        |
| Methane                       | 1.207                                | 12.51             | 1133                                                       |
| Methanethiol                  | 9.108(5)                             | 9.440(5)          | 888                                                        |
| Methanol                      | 1.047(1)                             | 10.85(1)          | 845                                                        |
| Methoxy                       | 0.83                                 | 8.6               | 845                                                        |
| Methoxybenzene (Anisole)      | 0.792(2)                             | 8.21(2)           | 724                                                        |
| 2-Methoxyethanol              | 0.93                                 | 9.6               | 562                                                        |
| Methyl                        | 0.949(1)                             | 9.84(1)           | 1095                                                       |
| Methyl acetate                | 0.991(2)                             | 10.27(2)          | 581                                                        |
| Methyl acrylate               | 0.96                                 | 9.9               | 611                                                        |
| Methyl azide                  | 0.947(2)                             | 9.81(2)           | 1227                                                       |
| Methyl benzoate               | 0.899(3)                             | 9.32(3)           | 611                                                        |
| Methyl chloroacetate          | 0.99                                 | 10.3              | 575                                                        |
| Methyl 2,2-dimethylpropanoate | 0.955(4)                             | 9.90(4)           | 466                                                        |
| Methyl formate                | 1.0435(5)                            | 10.815(5)         | 688                                                        |
| Methyl pentanoate             | 1.00(2)                              | 10.4(2)           | 532                                                        |
| Methyl pentyl ether           | 0.933                                | 9.67              | 657                                                        |
| Methyl vinyl ether            | 0.862(2)                             | 8.93(2)           | 761                                                        |
| Methylacrylonitrile           | 0.998                                | 10.34             | 1127                                                       |
| Methylamine                   | 0.865(2)                             | 8.97(2)           | 843                                                        |
| 2-Methylaniline               | 0.718(2)                             | 7.44(2)           | 772                                                        |



**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                         | Ionization energy         |                   | $\Delta_f H$ (ion)<br>in kJ · mol <sup>-1</sup> |
|-------------------------------------------------|---------------------------|-------------------|-------------------------------------------------|
|                                                 | In MJ · mol <sup>-1</sup> | In electron volts |                                                 |
| 3-Methylaniline                                 | 0.724(2)                  | 7.50(2)           | 778                                             |
| 4-Methylaniline                                 | 0.698(2)                  | 7.24(2)           | 753                                             |
| <i>N</i> -Methylaniline                         | 0.707(2)                  | 7.33(2)           | 791                                             |
| Methylcyclohexane                               | 0.930                     | 9.64              | 775                                             |
| 1-Methylcyclohexanol                            | 0.95(2)                   | 9.8(2)            | 586                                             |
| Methylcyclopentane                              | 0.950(3)                  | 9.85(3)           | 845                                             |
| Methylcyclopropane                              | 0.913                     | 9.46              | 936                                             |
| 2-Methyldecane                                  | 0.934                     | 9.68              | 685                                             |
| Methylene                                       | 1.0031(3)                 | 10.396(3)         | 1386                                            |
| <i>N</i> -Methylformamide                       | 0.945                     | 9.79              | 756                                             |
| 2-Methylheptane                                 | 0.949                     | 9.84              | 734                                             |
| 5-Methyl-2-hexanone                             | 0.895(1)                  | 9.28(1)           | 586                                             |
| Methylhydrazine                                 | 0.740(2)                  | 7.67(2)           | 835                                             |
| Methylidyne                                     | 1.027(1)                  | 10.64(1)          | 1622                                            |
| Methylisocyanate                                | 1.030(2)                  | 10.67(2)          | 900                                             |
| 1-Methyl-4-isopropylbenzene ( <i>p</i> -Cymene) | 0.800                     | 8.29              | 771                                             |
| 1-Methylnaphthalene                             | 0.757                     | 7.85              | 870                                             |
| 2-Methylnaphthalene                             | 0.75                      | 7.8               | 866                                             |
| Methyloxirane                                   | 0.986(2)                  | 10.22(2)          | 892                                             |
| 2-Methylpentane                                 | 0.976                     | 10.12             | 802                                             |
| 3-Methylpentane                                 | 0.973                     | 10.08             | 801                                             |
| 2-Methyl-3-pentanone                            | 0.878(1)                  | 9.10(1)           | 592                                             |
| 3-Methyl-2-pentanone                            | 0.889(1)                  | 9.21(1)           | 600                                             |
| 4-Methyl-2-pentanone                            | 0.897(1)                  | 9.30(1)           | 609                                             |
| 2-Methyl-1-pentene                              | 0.876(1)                  | 9.08(1)           | 817                                             |
| 2-Methyl-2-pentene                              | 0.828                     | 8.58              | 761                                             |
| 4-Methyl-1-pentene                              | 0.912(1)                  | 9.45(1)           | 862                                             |
| 4-Methyl- <i>cis</i> -2-pentene                 | 0.866(1)                  | 8.98(1)           | 809                                             |
| 4-Methyl- <i>trans</i> -2-pentene               | 0.865(1)                  | 8.97(1)           | 804                                             |
| 2-Methylpropanal                                | 0.9364(5)                 | 9.705(5)          | 721                                             |
| 2-Methylpropanenitrile                          | 1.09                      | 11.3              | 1115                                            |
| 2-Methylpropenal                                | 0.951                     | 9.86              | 834                                             |
| 2-Methylpropene (Isobutene)                     | 0.8915(3)                 | 9.239(3)          | 875                                             |
| 2-Methylpyridine                                | 0.870(3)                  | 9.02(3)           | 970                                             |
| 3-Methylpyridine                                | 0.872(3)                  | 9.04(3)           | 979                                             |
| 4-Methylpyridine                                | 0.872(3)                  | 9.04(3)           | 976                                             |
| Methylsilane                                    | 1.03                      | 10.7              | 1003                                            |
| <i>m</i> -Methylstyrene                         | 0.786(2)                  | 8.15(2)           | 908                                             |
| <i>o</i> -Methylstyrene                         | 0.888(2)                  | 9.20(2)           | 908                                             |
| <i>p</i> -Methylstyrene                         | 0.78(1)                   | 8.1(1)            | 895                                             |
| Methyltrichlorosilane                           | 1.096(3)                  | 11.36(3)          | 548                                             |
| Naphthalene                                     | 0.785(1)                  | 8.14(1)           | 936                                             |
| 1-Naphthol                                      | 0.749(3)                  | 7.76(3)           | 719                                             |
| 2-Naphthol                                      | 0.757(5)                  | 7.85(5)           | 727                                             |
| Nickel carbonyl                                 | 0.798(4)                  | 8.27(4)           | 200                                             |
| <i>m</i> -Nitroaniline                          | 0.802(2)                  | 8.31(2)           | 865                                             |
| <i>o</i> -Nitroaniline                          | 0.798(1)                  | 8.27(1)           | 861                                             |
| <i>p</i> -Nitroaniline                          | 0.804(1)                  | 8.34(1)           | 850                                             |
| Nitrobenzene                                    | 0.951(2)                  | 9.86(2)           | 1019                                            |
| Nitroethane                                     | 1.050(5)                  | 10.88(5)          | 948                                             |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                      | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                              | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Nitromethane                 | 1.063(4)                             | 11.02(4)          | 988                                                        |
| <i>m</i> -Nitrophenol        | 0.86                                 | 9.0               | 755                                                        |
| <i>o</i> -Nitrophenol        | 0.88                                 | 9.1               | 782                                                        |
| <i>p</i> -Nitrophenol        | 0.88                                 | 9.1               | 761                                                        |
| 1-Nitropropane               | 1.043(3)                             | 10.81(3)          | 919                                                        |
| 2-Nitropropane               | 1.033(5)                             | 10.71(5)          | 894                                                        |
| <i>m</i> -Nitrotoluene       | 0.15(2)                              | 9.48(2)           | 944                                                        |
| <i>o</i> -Nitrotoluene       | 0.912(4)                             | 9.45(4)           | 966                                                        |
| <i>p</i> -Nitrotoluene       | 0.91                                 | 9.4               | 936                                                        |
| Nonane                       | 0.938                                | 9.72              | 710                                                        |
| 2-Nonanone                   | 0.884                                | 9.16              | 545                                                        |
| 5-Nonanone                   | 0.875                                | 9.07              | 530                                                        |
| Octafluoronaphthalene        | 0.854                                | 8.85              | − 368                                                      |
| Octafluoropropane            | 1.291                                | 13.38             | − 491                                                      |
| Octafluorotoluene            | 0.96                                 | 9.9               | − 233                                                      |
| Octane                       | 0.948                                | 9.82              | 739                                                        |
| 1-Octene                     | 0.910(1)                             | 9.43(1)           | 829                                                        |
| 1-Octyne                     | 0.960(2)                             | 9.95(2)           | 1040                                                       |
| 2-Octyne                     | 0.898(1)                             | 9.31(1)           | 961                                                        |
| 3-Octyne                     | 0.890(1)                             | 9.22(1)           | 952                                                        |
| 4-Octyne                     | 0.888(1)                             | 9.20(1)           | 946                                                        |
| Oxazole                      | 0.93                                 | 9.6               | 910                                                        |
| Oxetane                      | 0.9328(5)                            | 9.668(5)          | 853                                                        |
| 2-Oxetanone                  | 0.936(1)                             | 9.70(1)           | 653                                                        |
| Oxomethyl (HCO)              | 0.782(5)                             | 8.10(5)           | 826                                                        |
| Pentafluorobenzene           | 0.929                                | 9.63              | 122                                                        |
| Pentafluorophenol            | 0.888(2)                             | 9.20(2)           | − 71                                                       |
| 2,3,4,5,6-Pentafluorotoluene | 0.91                                 | 9.4               | 64                                                         |
| Pentachloroethane            | 1.06                                 | 11.0              | 919                                                        |
| Pentylamine                  | 0.837                                | 8.67              | 728                                                        |
| Perylene                     | 0.666(1)                             | 6.90(1)           | 975                                                        |
| Phenanthrene                 | 0.758(2)                             | 7.86(2)           | 963                                                        |
| Phenetole                    | 0.784(2)                             | 8.13(2)           | 683                                                        |
| Phenol                       | 0.817                                | 8.47              | 721                                                        |
| Phenylacetic acid            | 0.797                                | 8.26              | 479                                                        |
| <i>m</i> -Phenylenediamine   | 0.689                                | 7.14              | 777                                                        |
| <i>o</i> -Phenylenediamine   | 0.69                                 | 7.2               | 787                                                        |
| <i>p</i> -Phenylenediamine   | 0.663(5)                             | 6.87(5)           | 759                                                        |
| Phthalic anhydride           | 0.96                                 | 10.0              | 593                                                        |
| $\alpha$ -Pinene             | 0.779                                | 8.07              | 808                                                        |
| Propanal                     | 0.9603(5)                            | 9.953(5)          | 773                                                        |
| Propanamide                  | 0.92                                 | 9.5               | 720                                                        |
| Propane                      | 1.057(5)                             | 10.95(5)          | 952                                                        |
| Propanenitrile               | 1.142(2)                             | 11.84(2)          | 1194                                                       |
| 1-Propanethiol               | 0.8872(5)                            | 9.195(5)          | 819                                                        |
| 2-Propanethiol               | 0.882                                | 9.14              | 806                                                        |
| Propanoic acid               | 1.0155(3)                            | 10.525(3)         | 568                                                        |
| 1-Propanol                   | 0.986(3)                             | 10.22(3)          | 731                                                        |
| 2-Propanol                   | 0.976(8)                             | 10.12(8)          | 704                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                        | Ionization energy         |                   | $\Delta_f H$ (ion)<br>in kJ · mol <sup>-1</sup> |
|--------------------------------|---------------------------|-------------------|-------------------------------------------------|
|                                | In MJ · mol <sup>-1</sup> | In electron volts |                                                 |
| Propenal                       | 0.975(6)                  | 10.103(6)         | 900                                             |
| Propene                        | 0.939(2)                  | 9.73(2)           | 959                                             |
| Propenenitrile                 | 1.053(1)                  | 10.91(1)          | 1237                                            |
| Propenoic acid                 | 1.023                     | 10.60             | 701                                             |
| 1-Propylamine                  | 0.847(2)                  | 8.78(2)           | 777                                             |
| 2-Propylamine                  | 0.841(3)                  | 8.72(3)           | 758                                             |
| Propylbenzene                  | 0.841(1)                  | 8.72(1)           | 849                                             |
| Propylcyclohexane              | 0.913                     | 9.46              | 720                                             |
| Propylcyclopentane             | 0.965(4)                  | 10.00(4)          | 817                                             |
| Propyleneimine                 | 0.87                      | 9.0               | 960                                             |
| Propynal                       | 1.04                      | 10.8              | 1155                                            |
| Propyne                        | 1.000(1)                  | 10.36(1)          | 1186                                            |
| 2-Propyn-1-ol                  | 1.014                     | 10.51             | 1060                                            |
| Pyrene                         | 0.715                     | 7.41              | 933                                             |
| Pyridazine                     | 0.834                     | 8.64              | 1112                                            |
| Pyrimidine                     | 0.891                     | 9.23              | 1087                                            |
| Pyrrole                        | 0.7920(5)                 | 8.208(5)          | 900                                             |
| 2-Pyrrolidone                  | 0.89                      | 9.2               | 674                                             |
| Quinoline                      | 0.832(1)                  | 8.62(1)           | 1041                                            |
| <i>cis</i> -Stilbene           | 0.753(2)                  | 7.80(2)           | 1005                                            |
| <i>trans</i> -Stilbene         | 0.743(3)                  | 7.70(3)           | 977                                             |
| Styrene                        | 0.813(6)                  | 8.43(6)           | 961                                             |
| Succinic anhydride             | 1.02                      | 10.6              | 500                                             |
| Succinonitrile                 | 1.158(24)                 | 12.10(25)         | 1377                                            |
| Terephthalic acid              | 0.951(20)                 | 9.86(20)          | 232                                             |
| <i>m</i> -Terphenyl            | 0.773(1)                  | 8.01(1)           | 1057                                            |
| <i>o</i> -Terphenyl            | 0.77                      | 8.0               | 1056                                            |
| <i>p</i> -Terphenyl            | 0.751(1)                  | 7.78(1)           | 1035                                            |
| Tetrabromomethane              | 0.995(2)                  | 10.31(2)          | 1079                                            |
| Tetrachloro-1,2-difluoroethane | 1.09                      | 11.3              | 563                                             |
| 1,1,1,2-Tetrachloroethane      | 1.07                      | 11.1              | 920                                             |
| 1,1,2,2-Tetrachloroethane      | 1.121                     | 11.62             | 971                                             |
| Tetrachloroethylene            | 0.899                     | 9.32              | 887                                             |
| Tetrachloromethane             | 1.107(1)                  | 11.47(1)          | 1011                                            |
| Tetraethylsilane               | 0.86                      | 8.9               | 595                                             |
| 1,2,3,4-Tetrafluorobenzene     | 0.920(1)                  | 9.53(1)           | 284                                             |
| 1,2,3,5-Tetrafluorobenzene     | 0.920(1)                  | 9.53(1)           | 263                                             |
| 1,2,4,5-Tetrafluorobenzene     | 0.902(1)                  | 9.35(1)           | 254                                             |
| Tetrafluoroethylene            | 0.976(2)                  | 10.12(2)          | 315                                             |
| Tetrahydrofurane               | 0.908(2)                  | 9.41(2)           | 724                                             |
| 1,2,3,4-Tetrahydronaphthalene  | 0.817                     | 8.47              | 842                                             |
| 1,2,4,5-Tetramethylbenzene     | 0.776(1)                  | 8.04(1)           | 730                                             |
| 2,2,3,3-Tetramethylbutane      | 0.95                      | 9.8               | 720                                             |
| Thiacyclobutane                | 0.838                     | 8.69              | 899                                             |
| Thiophene                      | 0.856(4)                  | 8.87(4)           | 971                                             |
| <i>p</i> -Tolualdehyde         | 0.900(5)                  | 9.33(5)           | 825                                             |
| Toluene                        | 0.851(1)                  | 8.82(1)           | 901                                             |
| <i>m</i> -Toluic acid          | 0.910(20)                 | 9.43(20)          | 579                                             |
| <i>o</i> -Toluic acid          | 0.88                      | 9.1               | 558                                             |
| <i>p</i> -Toluic acid          | 0.891(20)                 | 9.23(20)          | 560                                             |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|----------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                        | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| <i>m</i> -Tolunitrile                  | 0.901                                | 9.34              | 1085                                                       |
| <i>o</i> -Tolunitrile                  | 0.905                                | 9.38              | 1085                                                       |
| <i>p</i> -Tolunitrile                  | 0.899                                | 9.32              | 1083                                                       |
| Tribromomethane                        | 1.011(2)                             | 10.48(2)          | 1035                                                       |
| Tributylamine                          | 0.71                                 | 7.4               | 492                                                        |
| Trichloroacetyl chloride               | 1.06                                 | 11.0              | 827                                                        |
| 1,2,4-Trichlorobenzene                 | 0.872                                | 9.04              | 880                                                        |
| 1,3,5-Trichlorobenzene                 | 0.899(2)                             | 9.32(2)           | 899                                                        |
| 1,1,1-Trichloroethane                  | 1.06                                 | 11.0              | 917                                                        |
| 1,1,2-Trichloroethane                  | 1.06                                 | 11.0              | 911                                                        |
| Trichloroethylene                      | 0.914(1)                             | 9.47(1)           | 895                                                        |
| Trichlorofluoromethane                 | 1.136(2)                             | 11.77(2)          | 868                                                        |
| Trichloromethane                       | 1.097(2)                             | 11.37(2)          | 992                                                        |
| Trichloromethylbenzene                 | 0.926                                | 9.60              | 914                                                        |
| 1,1,2-Trichlorotrifluoroethane         | 1.157(2)                             | 11.99(2)          | 429                                                        |
| Triethanolamine                        | 0.76                                 | 7.9               | 206                                                        |
| Triethylamine                          | 0.724                                | 7.50              | 631                                                        |
| Trifluoroacetic acid                   | 1.106                                | 11.46             | 75                                                         |
| Trifluoroacetonitrile                  | 1.337                                | 13.86             | 838                                                        |
| 1,1,1-Trifluoro-2-bromo-2-chloroethane | 1.06                                 | 11.0              | 362                                                        |
| 1,1,1-Trifluoroethane                  | 1.24(1)                              | 12.9(1)           | 496                                                        |
| Trifluoroethylene                      | 0.978                                | 10.14             | 489                                                        |
| Trifluoriodomethane                    | 0.987                                | 10.23             | 397                                                        |
| Trifluoromethane                       | 1.337                                | 13.86             | 643                                                        |
| Trifluoromethyl ( $\text{CF}_3$ )      | 0.86                                 | 8.9               | 399                                                        |
| Trifluoromethylbenzene                 | 0.9345(4)                            | 9.685(4)          | 335                                                        |
| 3,3,3-Trifluoropropene                 | 1.05                                 | 10.9              | 437                                                        |
| Triiodomethane                         | 0.893(2)                             | 9.25(2)           | 1010                                                       |
| Trimethylamine                         | 0.755462                             | 7.82960           | 731                                                        |
| 1,2,3-Trimethylbenzene                 | 0.812(2)                             | 8.42(2)           | 803                                                        |
| 1,2,4-Trimethylbenzene                 | 0.798(1)                             | 8.27(1)           | 784                                                        |
| 1,3,5-Trimethylbenzene                 | 0.811(1)                             | 8.41(1)           | 796                                                        |
| Trimethylborate                        | 0.96                                 | 10.0              | 65                                                         |
| Trimethylchlorosilane                  | 0.979                                | 10.15             | 624                                                        |
| 3,5,5-Trimethylcyclohex-2-en-1-one     | 0.875                                | 9.07              | 670                                                        |
| 2,2,4-Trimethylpentane                 | 0.951                                | 9.86              | 713                                                        |
| 2,2,4-Trimethyl-3-pentanone            | 0.849(1)                             | 8.80(1)           | 511                                                        |
| 2,4,6-Trimethylpyridine                | 0.88(1)                              | 8.9(1)            | 580                                                        |
| Trioxane                               | 0.99                                 | 10.3              | 528                                                        |
| Undecane                               | 0.922                                | 9.56              | 650                                                        |
| Urea                                   | 0.94                                 | 9.7               | 690                                                        |
| Vinyl acetate                          | 0.887                                | 9.19              | 572                                                        |
| <i>m</i> -Xylene                       | 0.826(1)                             | 8.56(1)           | 843                                                        |
| <i>o</i> -Xylene                       | 0.826(1)                             | 8.56(1)           | 844                                                        |
| <i>p</i> -Xylene                       | 0.814(1)                             | 8.44(1)           | 832                                                        |
| 2,3-Xylenol                            | 0.797                                | 8.26              | 640                                                        |
| 2,4-Xylenol                            | 0.77                                 | 8.0               | 609                                                        |
| 2,6-Xylenol                            | 0.777(2)                             | 8.05(2)           | 615                                                        |
| 3,4-Xylenol                            | 0.781                                | 8.09              | 624                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)  
*Inorganic compounds*

| Species                                        | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|------------------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                                | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Aluminum tribromide                            | 1.00                                 | 10.4              | 593                                                        |
| Aluminum trichloride                           | 1.159                                | 12.01             | 573                                                        |
| Aluminum trifluoride                           | 1.394                                | 14.45             | 282                                                        |
| Aluminum triiodide                             | 0.88                                 | 9.1               | 673                                                        |
| Amidogen ( $\text{NH}_2$ )                     | 1.075(1)                             | 11.14(1)          | 1264                                                       |
| Ammonia                                        | 0.980(1)                             | 10.16(1)          | 934                                                        |
| Antimony trichloride                           | 0.97(1)                              | 10.1(1)           | 661                                                        |
| Arsenic trichloride                            | 1.018(3)                             | 10.55(3)          | 754                                                        |
| Arsenic trifluoride                            | 1.239(5)                             | 12.84(5)          | 452                                                        |
| Arsine                                         | 0.954                                | 9.89              | 1021                                                       |
| Barium oxide                                   | 0.667(6)                             | 6.91(6)           | 543                                                        |
| Bismuth trichloride                            | 1.00                                 | 10.4              | 736                                                        |
| Borane ( $\text{BH}_3$ )                       | 1.19(1)                              | 12.3(1)           | 1287                                                       |
| Boron dioxide ( $\text{BO}_2$ )                | 1.30(3)                              | 13.5(3)           | 1001                                                       |
| Boron oxide ( $\text{B}_2\text{O}_3$ )         | 1.303(14)                            | 13.50(15)         | 460                                                        |
| Boron tribromide                               | 1.014(2)                             | 10.51(2)          | 809                                                        |
| Boron trichloride                              | 1.119(2)                             | 11.60(2)          | 718                                                        |
| Boron trifluoride                              | 1.501(3)                             | 15.56(3)          | 365                                                        |
| Boron triiodide                                | 0.893(3)                             | 9.25(3)           | 964                                                        |
| Bromine ( $\text{Br}_2$ )                      | 1.0146(5)                            | 10.515(5)         | 1046                                                       |
| Bromine chloride ( $\text{BrCl}$ )             | 1.062                                | 11.01             | 1079                                                       |
| Bromine fluoride ( $\text{BrF}$ )              | 1.136(1)                             | 11.77(1)          | 1077                                                       |
| Bromine pentafluoride                          | 1.271(1)                             | 13.17(1)          | 840                                                        |
| Bromosilane ( $\text{BrSiH}_3$ )               | 1.02                                 | 10.6              | 943                                                        |
| Calcium oxide                                  | 0.67                                 | 6.9               | 691                                                        |
| Cesium chloride                                | 0.756(5)                             | 7.84(5)           | 510                                                        |
| Cesium fluoride                                | 1.221(1)                             | 12.65(1)          | 1170                                                       |
| Cesium fluoride                                | 0.849(10)                            | 8.80(10)          | 489                                                        |
| Chlorine ( $\text{Cl}_2$ )                     | 1.1424(5)                            | 11.840(5)         | 1108                                                       |
| Chlorine difluoride                            | 1.232(5)                             | 12.77(5)          | 1128                                                       |
| Chlorine dioxide                               | 1.000(2)                             | 10.36(2)          | 1096                                                       |
| Chlorine oxide                                 | 1.057                                | 10.95             | 1159                                                       |
| Chlorine trifluoride                           | 1.221(5)                             | 12.65(5)          | 1057                                                       |
| Chlorosilane ( $\text{ClSiH}_3$ )              | 1.10                                 | 11.4              | 899                                                        |
| Chromyl chloride ( $\text{CrO}_2\text{Cl}_2$ ) | 1.12                                 | 11.6              | 580                                                        |
| Diborane ( $\text{B}_2\text{H}_6$ )            | 1.098(3)                             | 11.38(3)          | 1134                                                       |
| Dichlorosilane ( $\text{Cl}_2\text{SiH}_2$ )   | 1.10                                 | 11.4              | 765                                                        |
| Difluoramine ( $\text{HNF}_2$ )                | 1.112(8)                             | 11.53(8)          | 1046                                                       |
| Difluoroamidogen ( $\text{NF}_2$ )             | 1.122(1)                             | 11.628(1)         | 1155                                                       |
| Difluorosilane ( $\text{F}_2\text{SiH}_2$ )    | 1.18                                 | 12.2              | 386                                                        |
| Dioxygen fluoride                              | 1.22(2)                              | 12.6(2)           | 1228                                                       |
| Disilane                                       | 0.94                                 | 9.7               | 1015                                                       |
| Disulfur oxide                                 | 1.017(4)                             | 10.54(4)          | 967                                                        |
| Fluorine ( $\text{F}_2$ )                      | 1.5146(3)                            | 15.697(3)         | 1515                                                       |
| Fluorosilane ( $\text{FSiH}_3$ )               | 1.13                                 | 11.7              | 752                                                        |
| Gallium bromide                                | 1.003                                | 10.40             | 711                                                        |
| Gallium chloride                               | 1.112                                | 11.52             | 648                                                        |
| Gallium triiodide                              | 0.907                                | 9.40              | 765                                                        |
| Gallium(I) fluoride                            | 0.93(5)                              | 9.6(5)            | 700                                                        |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                  | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|------------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                          | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Germane ( $\text{GeH}_4$ )               | 1.093                                | 11.33             | 1185                                                       |
| Germanium oxide ( $\text{GeO}$ )         | 1.085(1)                             | 11.25(1)          | 1044                                                       |
| Germanium sulfide ( $\text{GeS}$ )       | 0.963(2)                             | 9.98(2)           | 1055                                                       |
| Germanium tetrachloride                  | 1.1270(5)                            | 11.68(5)          | 629                                                        |
| Germanium tetrafluoride                  | 1.50                                 | 15.5              | 307                                                        |
| Germanium tetraiodide                    | 0.909                                | 9.42              | 850                                                        |
| Hafnium bromide                          | 1.05                                 | 10.9              | 366                                                        |
| Hafnium chloride                         | 1.13                                 | 11.7              | 246                                                        |
| Hexaborane ( $\text{B}_6\text{H}_{10}$ ) | 0.87                                 | 9.0               | 965                                                        |
| Hydrazine                                | 7.82(14)                             | 8.10(15)          | 877                                                        |
| Hydrazoic acid ( $\text{HN}_3$ )         | 1.0344(24)                           | 10.720(25)        | 1328                                                       |
| Hydrogen ( $\text{H}_2$ )                | 1.488413(5)                          | 15.42589(5)       | 1488                                                       |
| Hydrogen bromide                         | 1.125(3)                             | 11.66(3)          | 1087                                                       |
| Hydrogen chloride                        | 1.2299                               | 12.747            | 1137                                                       |
| Hydrogen fluoride                        | 1.5481(3)                            | 16.044(3)         | 1276                                                       |
| Hydrogen iodide                          | 1.0004(1)                            | 10.368(1)         | 1028                                                       |
| Hydrogen peroxide                        | 1.017                                | 10.54             | 881                                                        |
| Hydrogen selenide                        | 0.9535(1)                            | 9.882(1)          | 983                                                        |
| Hydrogen sulfide                         | 1.0085(8)                            | 10.453(8)         | 988                                                        |
| Hydroperoxy ( $\text{HOO}$ )             | 1.095(1)                             | 11.35(1)          | 1106                                                       |
| Hydroxyl ( $\text{OH}$ )                 | 1.254                                | 13.00             | 1293                                                       |
| Hydroxylamine ( $\text{NH}_2\text{OH}$ ) | 0.947                                | 10.00             | 923                                                        |
| Hypochlorous acid ( $\text{HOCl}$ )      | 1.073(1)                             | 11.12(1)          | 993                                                        |
| Hypofluorous acid ( $\text{HOF}$ )       | 1.226(1)                             | 12.71(1)          | 1130                                                       |
| Imidogen ( $\text{NH}$ )                 | 1.302(1)                             | 13.49(1)          | 1678                                                       |
| Iodine ( $\text{I}_2$ )                  | 0.90694(12)                          | 9.3995(12)        | 969                                                        |
| Iodine bromide                           | 0.9446(4)                            | 9.790(4)          | 986                                                        |
| Iodine chloride                          | 0.9734(10)                           | 10.088(10)        | 991                                                        |
| Iodine fluoride                          | 1.025                                | 10.62             | 930                                                        |
| Iodine pentafluoride                     | 1.2488(5)                            | 12.943(5)         | 408                                                        |
| Lead oxide ( $\text{PbO}$ )              | 0.976(10)                            | 9.08(10)          | 939                                                        |
| Lead(II) chloride                        | 0.96                                 | 10.0              | 789                                                        |
| Lead(II) fluoride                        | 1.11                                 | 11.5              | 679                                                        |
| Lead(II) sulfide                         | 0.825                                | 8.5(5)            | 954                                                        |
| Lithium bromide                          | 0.84                                 | 8.7               | 685                                                        |
| Lithium chloride                         | 0.923                                | 9.57              | 727                                                        |
| Lithium hydride                          | 0.74                                 | 7.7               | 882                                                        |
| Lithium iodide                           | 0.72                                 | 7.5               | 633                                                        |
| Lithium oxide                            | 0.815                                | 8.45(20)          | 895                                                        |
| Magnesium fluoride                       | 1.29                                 | 13.4              | 569                                                        |
| Magnesium oxide                          | 0.93                                 | 9.7               | 992                                                        |
| Mercapto ( $\text{SH}$ )                 | 1.001                                | 10.37             | 1140                                                       |
| Mercury(II) bromide                      | 1.019(3)                             | 10.560(3)         | 935                                                        |
| Mercury(II) chloride                     | 1.0988(3)                            | 11.380(3)         | 952                                                        |
| Mercury(II) iodide                       | 0.91748(22)                          | 9.5088(22)        | 900                                                        |
| Molybdenum hexafluoride                  | 1.40(1)                              | 14.5(1)           | − 159                                                      |
| Molybdenum(V) chloride                   | 0.84                                 | 8.7               | 392                                                        |
| Niobium(V) chloride                      | 1.058                                | 10.97             | 656                                                        |
| Nitric acid                              | 1.153(1)                             | 11.95(1)          | 1019                                                       |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                           | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|---------------------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                                   | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Nitric oxide                                      | 0.893900(6)                          | 9.26436(6)        | 985                                                        |
| Nitrogen ( $\text{N}_2$ )                         | 1.59336                              | 15.5808           | 1503                                                       |
| Nitrogen dioxide                                  | 0.941(1)                             | 9.75(1)           | 974                                                        |
| Nitrogen pentoxide                                | 1.15                                 | 11.9              | 1161                                                       |
| Nitrogen tetroxide                                | 1.04(2)                              | 10.8(2)           | 1050                                                       |
| Nitrogen trichloride                              | 0.9765(10)                           | 10.12(10)         | 1244                                                       |
| Nitrogen trifluoride                              | 1.254(2)                             | 13.00(2)          | 1125                                                       |
| Nitrosyl bromide                                  | 0.981(3)                             | 10.17(3)          | 1065                                                       |
| Nitrosyl chloride ( $\text{NOCl}$ )               | 1.049(1)                             | 10.87(1)          | 1099                                                       |
| Nitrosyl fluoride ( $\text{NOF}$ )                | 1.219(3)                             | 12.63(3)          | 1152                                                       |
| Nitrous acid ( $\text{HONO}$ )                    | 1.09                                 | 11.3              | 977                                                        |
| Nitrous oxide ( $\text{N}_2\text{O}$ )            | 1.2433                               | 12.886            | 1325                                                       |
| Nitryl chloride ( $\text{NO}_2\text{Cl}$ )        | 1.142                                | 11.84             | 1155                                                       |
| Nitryl fluoride ( $\text{NO}_2\text{F}$ )         | 1.263                                | 13.09             | 1154                                                       |
| Osmium tetroxide                                  | 1.1895                               | 12.320            | 850                                                        |
| Oxygen ( $\text{O}_2$ )                           | 1.1647(1)                            | 12.071(1)         | 1165                                                       |
| Oxygen dichloride                                 | 1.056                                | 10.94             | 1135                                                       |
| Oxygen difluoride ( $\text{OF}_2$ )               | 1.265(1)                             | 13.11(1)          | 1290                                                       |
| Oxygen fluoride                                   | 1.232                                | 12.77             | 1341                                                       |
| Ozone ( $\text{O}_3$ )                            | 1.199                                | 12.43             | 1342                                                       |
| Pentaborane ( $\text{B}_5\text{H}_9$ )            | 0.955(4)                             | 9.90(4)           | 1028                                                       |
| Perchloryl fluoride ( $\text{ClO}_3\text{F}$ )    | 1.2490(5)                            | 12.945(5)         | 1224                                                       |
| Phosphine ( $\text{PH}_3$ )                       | 0.9522(2)                            | 9.869(2)          | 958                                                        |
| Phosphorus ( $\text{P}_2$ )                       | 1.016                                | 10.53             | 1160                                                       |
| Phosphorus nitride                                | 1.143                                | 11.85             | 1248                                                       |
| Phosphorus pentachloride                          | 1.03                                 | 10.7              | 656                                                        |
| Phosphorus pentafluoride                          | 1.46                                 | 15.1              | − 137                                                      |
| Phosphorus sulfur trichloride ( $\text{PSCl}_3$ ) | 0.956                                | 9.91              | 668                                                        |
| Phosphorus tribromide                             | 0.94                                 | 9.7               | 798                                                        |
| Phosphorus trichloride                            | 0.956                                | 9.91              | 668                                                        |
| Phosphorus trifluoride                            | 1.104                                | 11.44             | 146                                                        |
| Phosphoryl chloride ( $\text{POCl}_3$ )           | 1.096(2)                             | 11.36(2)          | 540                                                        |
| Phosphoryl trifluoride ( $\text{POF}_3$ )         | 1.231(1)                             | 12.76(1)          | − 24                                                       |
| Potassium bromide                                 | 0.757(10)                            | 7.85(10)          | 578                                                        |
| Potassium chloride                                | 0.77(4)                              | 8.0(4)            | 557                                                        |
| Potassium iodide                                  | 0.696(29)                            | 7.21(30)          | 570                                                        |
| Rhenium(VII) oxide                                | 1.23(2)                              | 12.7(2)           | 125                                                        |
| Rubidium bromide                                  | 0.766(3)                             | 7.94(3)           | 583                                                        |
| Rubidium chloride                                 | 0.820(3)                             | 8.50(3)           | 590                                                        |
| Ruthenium tetroxide                               | 1.172(3)                             | 12.15(3)          | 988                                                        |
| Silane                                            | 1.124                                | 11.65             | 1158                                                       |
| Silicon oxide ( $\text{SiO}$ )                    | 1.103                                | 11.43             | 1002                                                       |
| Silicon tetrachloride                             | 1.136(1)                             | 11.79(1)          | 527                                                        |
| Silicon tetrafluoride                             | 1.51                                 | 15.7              | − 100                                                      |
| Silver chloride                                   | 0.973                                | 10.08             | 1065                                                       |
| Silver fluoride                                   | 1.06(3)                              | 11.0(3)           | 1071                                                       |
| Sodium bromide                                    | 0.802(10)                            | 8.31(10)          | 660                                                        |
| Sodium chloride                                   | 0.861(6)                             | 8.92(6)           | 681                                                        |
| Sodium iodide                                     | 0.737(2)                             | 7.64(2)           | 659                                                        |
| Stibine ( $\text{SbH}_3$ )                        | 0.920(3)                             | 9.54(3)           | 1067                                                       |

**TABLE 4.3** Ionization Energy of Molecular and Radical Species (*Continued*)

| Species                                        | Ionization energy                    |                   | $\Delta_f H$ (ion)<br>in $\text{kJ} \cdot \text{mol}^{-1}$ |
|------------------------------------------------|--------------------------------------|-------------------|------------------------------------------------------------|
|                                                | In $\text{MJ} \cdot \text{mol}^{-1}$ | In electron volts |                                                            |
| Strontium oxide                                | 0.675(14)                            | 7.00(15)          | 662                                                        |
| Sulfur ( $\text{S}_2$ )                        | 0.9027(2)                            | 9.356(2)          | 1031                                                       |
| Sulfur chloride pentafluoride                  | 1.1921(5)                            | 12.335(5)         | 144                                                        |
| Sulfur dichloride                              | 0.912(3)                             | 9.45(3)           | 895                                                        |
| Sulfur difluoride                              | 0.973                                | 10.08             | 676                                                        |
| Sulfur dioxide                                 | 1.189(2)                             | 12.32(2)          | 892                                                        |
| Sulfur hexafluoride                            | 1.479(3)                             | 15.33(3)          | 259                                                        |
| Sulfur oxide (SO)                              | 0.996(2)                             | 10.32(2)          | 1001                                                       |
| Sulfur pentafluoride                           | 1.01(1)                              | 10.5(1)           | 97                                                         |
| Sulfur trioxide                                | 1.235(4)                             | 12.80(4)          | 839                                                        |
| Sulfuryl chloride ( $\text{SO}_2\text{Cl}_2$ ) | 1.163                                | 12.05             | 807                                                        |
| Sulfuryl fluoride ( $\text{SO}_2\text{F}_2$ )  | 1.110                                | 11.5              | 679                                                        |
| Tantalum(V) chloride                           | 1.069                                | 11.08             | 348                                                        |
| Tetraborane ( $\text{B}_4\text{H}_{10}$ )      | 1.038(4)                             | 10.76(4)          | 1105                                                       |
| Tetrafluorohydrazine (gauche)                  | 1.152(3)                             | 11.94(3)          | 1119                                                       |
| Thallium(I) bromide                            | 0.882(2)                             | 9.14(2)           | 844                                                        |
| Thallium(I) chloride                           | 0.936(3)                             | 9.70(3)           | 869                                                        |
| Thallium(I) fluoride                           | 1.015                                | 10.52             | 835                                                        |
| Thionitrosyl fluoride (NSF)                    | 1.111(4)                             | 11.51(4)          | 1090                                                       |
| Thionyl chloride                               | 1.058                                | 10.96             | 844                                                        |
| Thionyl fluoride                               | 1.182                                | 12.25             | 688                                                        |
| Thiophosphoryl trifluoride ( $\text{PSF}_3$ )  | 1.066(4)                             | 11.05(4)          | 58                                                         |
| Thorium(IV) oxide                              | 0.847(14)                            | 8.70(15)          | 342                                                        |
| Tin(II) bromide                                | 0.87                                 | 9.0               | 830                                                        |
| Tin(II) chloride                               | 0.965                                | 10.0              | 760                                                        |
| Tin(II) fluoride                               | 1.07                                 | 11.1              | 586                                                        |
| Tin(II) oxide                                  | 0.926(2)                             | 9.60(2)           | 944                                                        |
| Tin(II) sulfide                                | 0.85                                 | 8.8               | 966                                                        |
| Tin(IV) bromide                                | 1.02                                 | 10.6              | 709                                                        |
| Tin(IV) chloride                               | 1.146(5)                             | 11.88(5)          | 673                                                        |
| Tin(IV) hydride                                | 1.037                                | 10.75             | 1200                                                       |
| Titanium(IV) bromide                           | 0.99                                 | 10.3              | 375                                                        |
| Titanium(IV) chloride                          | 1.124(14)                            | 11.65(15)         | 363                                                        |
| Titanium(IV) oxide                             | 0.920(10)                            | 9.54(10)          | 623                                                        |
| <i>trans</i> -Difluorodiazine                  | 1.24                                 | 12.8              | 1315                                                       |
| Trifluorammine oxide ( $\text{NOF}_3$ )        | 1.279(1)                             | 13.26(1)          | 1116                                                       |
| Trifluorosilane ( $\text{F}_3\text{SiH}$ )     | 1.35                                 | 14.0              | 150                                                        |
| Trisilane                                      | 0.89                                 | 9.2               | 1009                                                       |
| Tungsten(VI) chloride                          | 0.92                                 | 9.5               | 348                                                        |
| Uranium hexafluoride                           | 1.350(10)                            | 14.00(10)         | −796                                                       |
| Uranium(IV) oxide                              | 5.2(1)                               | 5.4(1)            | 57                                                         |
| Uranium(VI) oxide                              | 1.01(5)                              | 10.5(5)           | 214                                                        |
| Vanadium(IV) chloride                          | 0.89                                 | 9.2               | 210                                                        |
| Vanadium(V) oxychloride ( $\text{VOCl}_3$ )    | 1.120                                | 11.61             | 425                                                        |
| Water                                          | 1.2170(10)                           | 12.612(10)        | 975                                                        |
| Xenon difluoride                               | 1.192(1)                             | 12.35(1)          | 1083                                                       |
| Xenon tetrafluoride                            | 1.221(10)                            | 12.65(10)         | 1016                                                       |
| Zirconium bromide                              | 1.03                                 | 10.7              | 388                                                        |
| Zirconium chloride                             | 1.08                                 | 11.2              | 392                                                        |

**Source:** Sharon, G., et al., *J. Phys. Chem. Ref. Data*, 17:Suppl. No. 1 (1988).



4.3 ELECTRON AFFINITY

TABLE 4.4 Electron Affinities of Atoms, Molecules, and Radicals

Electron affinity of an atom (molecule or radical) is defined as the energy difference between the lowest (ground) state of the neutral and the lowest state of the corresponding negative ion in the gas phase.

$A(g) + e^- = A^-(g)$

Data are limited to those negative ions which, by virtue of their positive electron affinity, are stable. Uncertainty in the final data figures is given in parentheses. Calculated values are enclosed in brackets.

| A. Atoms                                  |                    |                           |
|-------------------------------------------|--------------------|---------------------------|
| Atom                                      | Electron affinity, |                           |
|                                           | in eV              | in kJ · mol <sup>-1</sup> |
| Aluminum                                  | 0.441(10)          | 42.5(10)                  |
| Antimony                                  | 1.046(5)           | 100.9(5)                  |
| Arsenic                                   | 0.81(3)            | 78.(3)                    |
| Astatine                                  | [2.8(3)]           | [270.(30)]                |
| Barium                                    | [0.15]             | [14.]                     |
| Bismuth                                   | 0.946(10)          | 91.3(10)                  |
| Boron                                     | 0.277(10)          | 26.7(10)                  |
| Bromine                                   | 3.363590(3)        | 324.5367(3)               |
| Calcium                                   | 0.0185(25)         | 1.78(24)                  |
| Carbon                                    | 1.2629(3)          | 121.85(3)                 |
| Cesium                                    | 0.471626(25)       | 45.5048(24)               |
| Chlorine                                  | 3.61269            | 348.570                   |
| Chromium                                  | 0.666(12)          | 64.3(12)                  |
| Cobalt                                    | 0.662(3)           | 63.9(3)                   |
| Copper                                    | 1.235(5)           | 119.2(5)                  |
| Fluorine                                  | 3.401190(4)        | 328.1638(4)               |
| Francium                                  | [0.46]             | [44]                      |
| Gallium                                   | 0.30(15)           | 29.(15)                   |
| Germanium                                 | 1.233(3)           | 119.0(3)                  |
| Gold                                      | 2.30863(3)         | 222.748(3)                |
| Hafnium                                   | [≈ 0.]             | [≈ 0.]                    |
| Hydrogen                                  | 0.75195(19)        | 72.552(18)                |
| Hydrogen- <i>d</i> <sub>1</sub> deuterium | 0.75459(7)         | 72.807(7)                 |
| Indium                                    | 0.3(2)             | 29.(2)                    |
| Iodine                                    | 3.05904(1)         | 295.151(1)                |
| Iridium                                   | 1.565(8)           | 151.0(8)                  |
| Iron                                      | 0.151(3)           | 14.6(3)                   |
| Lanthanum                                 | [0.5(3)]           | [48.(30)]                 |
| Lead                                      | 0.364(8)           | 35.1(8)                   |
| Lithium                                   | 0.6180(5)          | 59.63(5)                  |
| Molybdenum                                | 0.748(2)           | 72.2(2)                   |
| Nickel                                    | 1.156(10)          | 111.5(10)                 |
| Niobium                                   | 0.893(25)          | 86.2(24)                  |
| Osmium                                    | [0.2(1)]           | [19.(10)]                 |
| Oxygen                                    | 1.4611103(7)       | 140.97523(7)              |
| Palladium                                 | 0.562(5)           | 54.2(5)                   |
| Phosphorus                                | 0.7465(3)          | 72.03(3)                  |
| Platinum                                  | 2.128(2)           | 205.3(2)                  |
| Polonium                                  | [1.9(3)]           | [183.(30)]                |

**TABLE 4.4** Electron Affinities of Atoms, Molecules, and Radicals (*Continued*)

| A. Atoms ( <i>continued</i> )                                                 |                    |                           |
|-------------------------------------------------------------------------------|--------------------|---------------------------|
| Atom                                                                          | Electron affinity, |                           |
|                                                                               | in eV              | in kJ · mol <sup>-1</sup> |
| Potassium                                                                     | 0.50147(10)        | 48.384(10)                |
| Rhenium                                                                       | [0.15(15)]         | [14.(14)]                 |
| Rubidium                                                                      | 0.48592(2)         | 46.884(2)                 |
| Ruthenium                                                                     | [1.05(15)]         | [101.(14)]                |
| Scandium                                                                      | 0.188(20)          | 18.1(19)                  |
| Selenium                                                                      | 2.020670(25)       | 194.9643(24)              |
| Silver                                                                        | 1.302(7)           | 125.6(7)                  |
| Sodium                                                                        | 0.547926(25)       | 52.86666(24)              |
| Strontium                                                                     | 0.048(6)           | 4.6(6)                    |
| Sulfur                                                                        | 2.077104(1)        | 200.4094(1)               |
| Tantalum                                                                      | 0.322(12)          | 31.1(12)                  |
| Technetium                                                                    | [0.55(20)]         | [53.(19)]                 |
| Tellurium                                                                     | 1.9708(3)          | 190.15(3)                 |
| Thallium                                                                      | 0.2(2)             | 19.(19)                   |
| Tin                                                                           | 1.112(4)           | 107.3(4)                  |
| Titanium                                                                      | 0.079(14)          | 7.6(14)                   |
| Tungsten                                                                      | 0.815(2)           | 78.6(2)                   |
| Vanadium                                                                      | 0.525(12)          | 50.7(12)                  |
| Yttrium                                                                       | 0.307(12)          | 29.6(12)                  |
| Zirconium                                                                     | 0.426(14)          | 41.1(14)                  |
| B. Molecules                                                                  |                    |                           |
| Molecule                                                                      | Electron affinity, |                           |
|                                                                               | in eV              | in kJ · mol <sup>-1</sup> |
| BF <sub>3</sub>                                                               | 2.65               | 256                       |
| BH <sub>3</sub>                                                               | 0.038(15)          | 3.7(15)                   |
| 1,4-Benzoquinone                                                              | 1.91(10)           | 184.(10)                  |
| Br <sub>2</sub>                                                               | 2.55(10)           | 246.(10)                  |
| CBrF <sub>3</sub>                                                             | 0.91(20)           | 89.(19)                   |
| CF <sub>3</sub> I                                                             | 1.57(20)           | 151.(19)                  |
| COS                                                                           | 0.46(20)           | 44.(19)                   |
| CS <sub>2</sub>                                                               | 0.895(20)          | 86.3(19)                  |
| C <sub>6</sub> F <sub>6</sub> hexafluorobenzene                               | 0.52(10)           | 50.(10)                   |
| 1,2-C <sub>6</sub> H <sub>4</sub> (NO <sub>2</sub> ) <sub>2</sub> (also 1,3-) | 1.65(10)           | 159.(10)                  |
| 1,4-C <sub>6</sub> H <sub>4</sub> (NO <sub>2</sub> ) <sub>2</sub>             | 2.00(10)           | 193.(10)                  |
| C <sub>6</sub> H <sub>5</sub> Br bromobenzene                                 | 1.15(11)           | 111.(11)                  |
| C <sub>6</sub> H <sub>5</sub> Cl chlorobenzene                                | 0.82(11)           | 79.(11)                   |
| C <sub>6</sub> H <sub>5</sub> I iodobenzene                                   | 1.41(11)           | 136.(11)                  |
| C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> nitrobenzene                    | 1.01(10)           | 97.(10)                   |
| 1,4-C <sub>6</sub> H <sub>4</sub> (CN)NO <sub>2</sub>                         | 1.72(10)           | 166.(10)                  |
| Cl <sub>2</sub>                                                               | 2.38(10)           | 229.(10)                  |
| CoH <sub>2</sub>                                                              | 1.450(14)          | 139.9(13)                 |
| CsCl                                                                          | 0.455(10)          | 43.9(10)                  |
| CuO                                                                           | 1.777(6)           | 171.5(6)                  |
| F <sub>2</sub>                                                                | 3.08(10)           | 297.(10)                  |
| FeO                                                                           | 1.493(5)           | 144.1(5)                  |
| I <sub>2</sub>                                                                | 2.55(5)            | 246.(5)                   |

**TABLE 4.4** Electron Affinities of Atoms, Molecules, and Radicals (*Continued*)

| B. Molecules ( <i>continued</i> ) |                    |                           |
|-----------------------------------|--------------------|---------------------------|
| Molecule                          | Electron affinity, |                           |
|                                   | in eV              | in kJ · mol <sup>-1</sup> |
| IBr                               | 2.55(10)           | 246.(10)                  |
| IrF <sub>6</sub>                  | 6.5(4)             | 627.(40)                  |
| KBr                               | 0.642(10)          | 61.9(10)                  |
| KCl                               | 0.582(10)          | 56.1(10)                  |
| KI                                | 0.728(10)          | 70.2(10)                  |
| LiCl                              | 0.593(10)          | 54.3(10)                  |
| LiH                               | 0.342(12)          | 33.0(12)                  |
| MoO <sub>3</sub>                  | 2.9(2)             | 280.(20)                  |
| NO                                | 0.026(5)           | 2.5(5)                    |
| NO <sub>2</sub>                   | 2.273(5)           | 219.3(5)                  |
| N <sub>2</sub> O                  | 0.22(10)           | 21.(10)                   |
| NaBr                              | 0.788(10)          | 76.0(10)                  |
| NaCl                              | 0.727(10)          | 70.1(10)                  |
| NaI                               | 0.865(10)          | 83.5(10)                  |
| NaK                               | 0.465(30)          | 44.9(30)                  |
| O <sub>2</sub>                    | 0.451(7)           | 43.5(7)                   |
| O <sub>3</sub>                    | 2.103(3)           | 202.9(9)                  |
| OsF <sub>6</sub>                  | 6.0(3)             | 579.(29)                  |
| PBr <sub>3</sub>                  | 1.59(15)           | 153.(14)                  |
| PCl <sub>3</sub>                  | 0.82(10)           | 79.(10)                   |
| PF <sub>5</sub>                   | 0.75(15)           | 72.(14)                   |
| POCl <sub>3</sub>                 | 1.41(2)            | 136.(2)                   |
| PbO                               | 0.722(6)           | 69.7(6)                   |
| PtF <sub>6</sub>                  | 7.0(4)             | 675.(40)                  |
| RbCl                              | 0.544(10)          | 52.5(10)                  |
| RuF <sub>6</sub>                  | 7.5(3)             | 724.(28)                  |
| SF <sub>4</sub>                   | 1.5(2)             | 145.(19)                  |
| SF <sub>6</sub>                   | 1.05(10)           | 101.(10)                  |
| SO <sub>2</sub>                   | 1.107(8)           | 106.8(8)                  |
| SeF <sub>6</sub>                  | 2.9(2)             | 280.(19)                  |
| SeO                               | 1.456(20)          | 140.5(19)                 |
| SeO <sub>2</sub>                  | 1.823(50)          | 175.9(48)                 |
| TeF <sub>6</sub>                  | 3.34(17)           | 322.(16)                  |
| TeO                               | 1.695(22)          | 163.5(21)                 |
| UF <sub>6</sub>                   | 5.1(2)             | 492.(19)                  |
| V <sub>4</sub> O <sub>10</sub>    | 4.2(6)             | 405.(60)                  |
| WO <sub>3</sub>                   | 3.9(2)             | 376.(19)                  |
| C. Radicals                       |                    |                           |
| Radical                           | Electron affinity, |                           |
|                                   | in eV              | in kJ · mol <sup>-1</sup> |
| AsH <sub>2</sub>                  | 1.27(3)            | 123.(3)                   |
| CCl <sub>2</sub>                  | 1.591(10)          | 153.5(10)                 |
| CF <sub>2</sub>                   | 0.165(10)          | 15.9(10)                  |
| CH                                | 1.238(8)           | 119.4(8)                  |
| CHBr                              | 1.454(5)           | 140.3(5)                  |
| CHCl                              | 1.210(5)           | 117.5(5)                  |
| CHF                               | 0.542(5)           | 52.3(5)                   |

**TABLE 4.4** Electron Affinities of Atoms, Molecules, and Radicals (*Continued*)

| Radical                                                             | Electron affinity, |                           |
|---------------------------------------------------------------------|--------------------|---------------------------|
|                                                                     | in eV              | in kJ · mol <sup>-1</sup> |
| CHI                                                                 | 1.42(17)           | 137.(17)                  |
| CHO <sub>2</sub>                                                    | 3.498(5)           | 337.5(5)                  |
| CH <sub>2</sub>                                                     | 0.652(6)           | 62.9(6)                   |
| CH <sub>2</sub> S                                                   | 0.465(23)          | 44.9(22)                  |
| CH <sub>2</sub> =SiH                                                | 2.010(10)          | 193.9(10)                 |
| CH <sub>3</sub>                                                     | 0.08(3)            | 7.7(3)                    |
| CH <sub>3</sub> CH <sub>2</sub> O ethoxide                          | 1.726(33)          | 166.5(32)                 |
| CH <sub>3</sub> O                                                   | 1.570(22)          | 151.5(21)                 |
| CH <sub>3</sub> S                                                   | 1.861(4)           | 179.6(4)                  |
| CH <sub>3</sub> SCH <sub>2</sub>                                    | 0.868(51)          | 83.7(49)                  |
| CH <sub>3</sub> Si                                                  | 0.852(10)          | 82.2(10)                  |
| CH <sub>3</sub> SiH <sub>2</sub>                                    | 1.19(4)            | 115.(4)                   |
| C <sub>2</sub> F <sub>2</sub> difluorovinylidene                    | 2.255(6)           | 217.6(6)                  |
| C <sub>2</sub> H <sub>2</sub> vinylidene                            | 0.490(6)           | 47.3(6)                   |
| CH <sub>2</sub> =CH vinyl                                           | 0.667(24)          | 64.3(23)                  |
| C <sub>2</sub> H <sub>3</sub> O acetaldehyde enolate                | 1.82476(12)        | 176.062(12)               |
| CH <sub>3</sub> CH <sub>2</sub> S                                   | 1.953(6)           | 188.4(6)                  |
| HC≡C—CH <sub>2</sub>                                                | 0.893(25)          | 86.2(24)                  |
| CH <sub>3</sub> CHCN                                                | 1.247(12)          | 120.3(12)                 |
| C <sub>2</sub> H <sub>5</sub> O ethoxide                            | 1.726(33)          | 166.5(31)                 |
| C <sub>2</sub> H <sub>5</sub> S ethyl sulfide                       | 1.953(6)           | 188.4(6)                  |
| C <sub>3</sub> H <sub>3</sub> propargyl radical                     | 0.893(25)          | 86.2(24)                  |
| CH <sub>3</sub> CH—CN                                               | 1.247(12)          | 120.3(12)                 |
| C <sub>3</sub> H <sub>5</sub> allyl                                 | 0.362(19)          | 34.9(18)                  |
| C <sub>3</sub> H <sub>5</sub> O acetone enolate                     | 1.758(19)          | 169.2(18)                 |
| propionaldehyde enolate                                             | 1.621(6)           | 156.4(6)                  |
| C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> methyl acetate enolate | 1.80(6)            | 174.(6)                   |
| C <sub>3</sub> H <sub>7</sub> O propoxide                           | 1.789(33)          | 172.6(31)                 |
| isopropyl oxide                                                     | 1.839(29)          | 177.4(28)                 |
| C <sub>3</sub> H <sub>7</sub> S propyl sulfide                      | 2.00(2)            | 193.(2)                   |
| isopropyl sulfide                                                   | 2.02(2)            | 195.(2)                   |
| C <sub>4</sub> H <sub>5</sub> O cyclobutanone enolate               | 1.801(8)           | 173.8(8)                  |
| C <sub>4</sub> H <sub>7</sub> O butyraldehyde enolate               | 1.67(5)            | 161.(5)                   |
| C <sub>4</sub> H <sub>9</sub> O <i>tert</i> -butoxyl                | 1.912(54)          | 184.5(52)                 |
| C <sub>4</sub> H <sub>9</sub> S butyl sulfide                       | 2.03(2)            | 196.(2)                   |
| <i>tert</i> -butyl sulfide                                          | 2.07(2)            | 200.(2)                   |
| C <sub>5</sub> H <sub>5</sub> cyclopentadienyl                      | 1.804(7)           | 174.1(7)                  |
| C <sub>5</sub> H <sub>7</sub> pentadienyl                           | 0.91(3)            | 88.(3)                    |
| C <sub>5</sub> H <sub>7</sub> O cyclopentanone enolate              | 1.598(7)           | 154.2(7)                  |
| C <sub>5</sub> H <sub>9</sub> O 3-pentanone enolate                 | 1.69(5)            | 163.(5)                   |
| C <sub>5</sub> H <sub>11</sub> S pentyl sulfide                     | 2.09(2)            | 202.(2)                   |
| C <sub>6</sub> H <sub>5</sub> phenyl                                | 1.096(6)           | 105.7(6)                  |
| C <sub>6</sub> H <sub>5</sub> NH anilide                            | 1.70(3)            | 164.(3)                   |
| C <sub>6</sub> H <sub>5</sub> O phenoxyl                            | 2.253(6)           | 217.4(6)                  |
| C <sub>6</sub> H <sub>5</sub> S thiophenoxide                       | ≤ 2.47(6)          | ≤ 238.(6)                 |
| C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> benzyl                | 0.912(6)           | 88.0(6)                   |
| C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> O benzyl oxide        | 2.14(2)            | 206.(2)                   |
| C <sub>6</sub> H <sub>9</sub> O cyclohexanone enolate               | 1.526(10)          | 147.2(10)                 |
| H <sub>2</sub> C=CH—CH=CH—CH=CH—CH <sub>2</sub> heptatrienyl        | 1.27(3)            | 122.(3)                   |
| CN                                                                  | 3.862(4)           | 372.6(4)                  |

**TABLE 4.4** Electron Affinities of Atoms, Molecules, and Radicals (*Continued*)

| Radical                       | C. Radicals ( <i>continued</i> ) |                           |
|-------------------------------|----------------------------------|---------------------------|
|                               | Electron affinity,               |                           |
|                               | in eV                            | in kJ · mol <sup>-1</sup> |
| CNCH <sub>2</sub> cyanomethyl | 1.543(14)                        | 148.9(14)                 |
| CO <sub>3</sub>               | 2.69(14)                         | 259.(14)                  |
| CS                            | 0.205(21)                        | 19.8(20)                  |
| ClO                           | 2.275(6)                         | 219.5(6)                  |
| HCO                           | 0.313(5)                         | 30.2(5)                   |
| HNO                           | 0.338(15)                        | 32.6(14)                  |
| HO <sub>2</sub>               | 1.078(17)                        | 104.0(6)                  |
| FO                            | 2.272(6)                         | 219.2(6)                  |
| N <sub>3</sub>                | 2.70(12)                         | 260.(12)                  |
| NCO                           | 3.609(5)                         | 348.2(5)                  |
| NCS                           | 3.537(5)                         | 341.3(5)                  |
| NH                            | 0.370(4)                         | 35.7(4)                   |
| NO <sub>3</sub>               | 3.937(14)                        | 379.9(14)                 |
| NS                            | 1.194(11)                        | 115.2(11)                 |
| O <sub>2</sub> Aryl           | 0.52(2)                          | 50.(2)                    |
| OCLO                          | 2.140(8)                         | 206.5(8)                  |
| OH                            | 1.82767(2)                       | 176.343(2)                |
| OIO                           | 2.577(8)                         | 248.6(8)                  |
| PH                            | 1.028(10)                        | 99.2(10)                  |
| PH <sub>2</sub>               | 1.27(1)                          | 123.(1)                   |
| PO                            | 1.092(10)                        | 105.4(10)                 |
| PO <sub>2</sub>               | 3.42(1)                          | 330.(1)                   |
| SF                            | 2.285(6)                         | 220.5(6)                  |
| SH                            | 2.314344(4)                      | 223.300(4)                |
| SO                            | 1.125(5)                         | 108.5(5)                  |
| SeH                           | 2.21252(3)                       | 213.475(3)                |
| SiF <sub>3</sub>              | ≤ 2.95(10)                       | 285.(10)                  |
| SiH                           | 1.277(9)                         | 123.2(9)                  |
| SiH <sub>2</sub>              | 1.124(20)                        | 108.4(19)                 |
| SiH <sub>3</sub>              | 1.406(14)                        | 106.7(14)                 |

**Source:** H. Hotop and W. C. Lineberger, *J. Phys. Chem. Reference Data* **14**:731 (1985).

4.4 ELECTRONEGATIVITY

Electronegativity  $\chi$  is the relative attraction of an atom for the valence electrons in a covalent bond. It is proportional to the effective nuclear charge and inversely proportional to the covalent radius:

$$\chi = \frac{0.31(n + 1 \pm c)}{r} + 0.50$$

where  $n$  is the number of valence electrons,  $c$  is any formal valence charge on the atom and the sign before it corresponds to the sign of this charge, and  $r$  is the covalent radius. Originally the element fluorine, whose atoms have the greatest attraction for electrons, was given an arbitrary electronegativity of 4.0. A revision of Pauling’s values based on newer data assigns 3.90 to fluorine. Values in Table 4.5 refer to the common oxidation states of the elements.

**TABLE 4.5** Electronegativities of the Elements

|                    |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |  |  |
|--------------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|--|--|
| H<br>2.20          |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |  |  |
| Li<br>0.98         | Be<br>1.57 |            |            |            |            |            |            |            |            |            |            | B<br>2.04  | C<br>2.55  | N<br>3.04  | O<br>3.44  | F<br>3.90  |  |  |
| Na<br>0.93         | Mg<br>1.31 |            |            |            |            |            |            |            |            |            |            | Al<br>1.61 | Si<br>1.90 | P<br>2.19  | S<br>2.58  | Cl<br>3.16 |  |  |
| K<br>0.82          | Ca<br>1.00 | Sc<br>1.36 | Ti<br>1.54 | V<br>1.63  | Cr<br>1.66 | Mn<br>1.55 | Fe<br>1.83 | Co<br>1.88 | Ni<br>1.91 | Cu<br>1.90 | Zn<br>1.65 | Ga<br>1.81 | Ge<br>2.01 | As<br>2.18 | Se<br>2.55 | Br<br>2.96 |  |  |
| Rb<br>0.82         | Sr<br>0.95 | Y<br>1.22  | Zr<br>1.33 | Nb<br>1.6  | Mo<br>2.16 | Tc<br>2.10 | Ru<br>2.2  | Rh<br>2.28 | Pd<br>2.20 | Ag<br>1.93 | Cd<br>1.69 | In<br>1.78 | Sn<br>1.96 | Sb<br>2.05 | Te<br>2.1  | I<br>2.66  |  |  |
| Cs<br>0.79         | Ba<br>0.89 | La<br>1.10 | Hf<br>1.3  | Ta<br>1.5  | W<br>1.7   | Re<br>1.9  | Os<br>2.2  | Ir<br>2.2  | Pt<br>2.2  | Au<br>2.4  | Hg<br>1.9  | Tl<br>1.8  | Pb<br>1.8  | Bi<br>1.9  | Po<br>2.0  | At<br>2.2  |  |  |
| Fr<br>0.7          | Ra<br>0.9  | Ac<br>1.1  |            |            |            |            |            |            |            |            |            |            |            |            |            |            |  |  |
| <i>Lanthanides</i> |            |            | Ce<br>1.12 | Pr<br>1.13 | Nd<br>1.14 | Sm<br>1.17 |            | Gd<br>1.20 |            | Dy<br>1.22 |            | Ho<br>1.23 | Er<br>1.24 | Tm<br>1.25 | Lu<br>1.0  |            |  |  |
| <i>Actinides</i>   |            |            | Th<br>1.3  | Pa<br>1.5  | U<br>1.7   | Np<br>1.3  | Pu<br>1.3  | Am<br>1.3  | Cm<br>1.3  | Bk<br>1.3  | Cf<br>1.3  | Es<br>1.3  | Fm<br>1.3  | Md<br>1.3  | No<br>1.3  |            |  |  |

**Source:** L. Pauling, *The Chemical Bond*, Cornell University Press, Ithaca, New York, 1967; L. C. Allen, *J. Am. Chem. Soc.* **111**:9003 (1989); A. L. Allred, *J. Inorg. Nucl. Chem.* **17**:215 (1961).

The greater the difference in electronegativity, the greater is the ionic character of the bond. The amount of ionic character  $I$  is given by:

$$I = 0.46 \left| \chi_A - \chi_B \right| + 0.035(\chi_A - \chi_B)^2$$

The bond is fully covalent when  $(\chi_A - \chi_B) < 0.5$  (and  $I < 6\%$ ).

## 4.5 BOND LENGTHS AND STRENGTHS

### 4.5.1 Atom Radius

The *atom radius* of an element is the shortest distance between like atoms. It is the distance of the centers of the atoms from one another in metallic crystals and for these materials the atom radius is often called the metal radius. Except for the lanthanides (CN = 6), CN = 12 for the elements. The atom radii listed in Table 4.6 are taken mostly from A. Kelly and G. W. Groves, *Crystallography and Crystal Defects*, Addison-Wesley, Reading, Mass., 1970.

TABLE 4.6 Atom Radii and Effective Ionic Radii of Elements

| Element     | Atom<br>radius,<br>pm | Effective ionic radii, pm |                     |       |       |     |
|-------------|-----------------------|---------------------------|---------------------|-------|-------|-----|
|             |                       | Ion<br>charge             | Coordination number |       |       |     |
|             |                       |                           | 4                   | 6     | 8     | 12  |
| Actinium    | 187.8                 | 3+                        |                     | 111   |       |     |
| Aluminum    | 143.1                 | 3+                        | 39                  | 53.5  |       |     |
| Americium   | 173                   | 2+                        |                     |       | 126   |     |
|             |                       | 3+                        |                     | 97.5  | 109   |     |
|             |                       | 4+                        |                     | 89    | 95    |     |
|             |                       | 5+                        |                     | 86    |       |     |
|             |                       | 6+                        |                     | 80    |       |     |
|             |                       | 3−                        |                     | 245   |       |     |
| Antimony    | 145                   | 1+                        |                     | 89    |       |     |
|             |                       | 3+                        | 76                  | 76    |       |     |
|             |                       | 5+                        |                     | 60    |       |     |
|             |                       | 3−                        |                     | 222   |       |     |
| Arsenic     | 124.8                 | 3+                        |                     | 58    |       |     |
|             |                       | 5+                        | 33.5                | 46    |       |     |
|             |                       | 1−                        |                     | 227   |       |     |
| Astatine    |                       | 5+                        |                     | 57    |       |     |
|             |                       | 7+                        |                     | 62    |       |     |
|             |                       | 2+                        |                     | 136   | 142   | 160 |
| Barium      | 217.3                 | 2+                        |                     | 118   |       |     |
| Berkelium   |                       | 3+                        |                     | 98    |       |     |
|             |                       | 4+                        |                     | 87    | 93    |     |
| Beryllium   | 111.3                 | 1−                        | 195                 |       |       |     |
| Bismuth     | 154.7                 | 2+                        | 27                  | 45    |       |     |
|             |                       | 3−                        |                     | 213   |       |     |
|             |                       | 3+                        |                     | 103   | 111   |     |
|             |                       | 5+                        |                     | 76    |       |     |
| Boron       | 86                    | 1+                        | 35                  |       |       |     |
|             |                       | 3+                        | 11                  | 27    |       |     |
| Bromine     |                       | 1−                        |                     | 196   |       |     |
|             |                       | 3+                        | 59                  |       |       |     |
|             |                       | 5+                        | 31*                 | 47    |       |     |
|             |                       | 7+                        |                     | 25    |       |     |
| Cadmium     | 148.9                 | 2+                        | 78                  | 95    | 110   | 131 |
| Calcium     | 197                   | 2+                        |                     | 100   | 112   | 135 |
| Californium | 186(2)                | 2+                        |                     | 117   |       |     |
|             |                       | 3+                        |                     | 95    |       |     |
|             |                       | 4+                        |                     | 82.1  |       |     |
|             |                       | 4−                        | 260                 |       |       |     |
| Carbon      |                       | 4+                        | 15                  | 16    |       |     |
| Cerium      | 181.8                 | 3+                        |                     | 102   | 114.3 | 134 |
|             |                       | 4+                        |                     | 87    | 97    | 114 |
| Cesium      | 265                   | 1+                        |                     | 167   | 174   | 188 |
| Chlorine    |                       | 1−                        |                     | 181   |       |     |
|             |                       | 5+                        | 34                  |       |       |     |
|             |                       | 7+                        | 8                   | 27    |       |     |
| Chromium    | 128                   | 1+                        | 81                  |       |       |     |
|             |                       | 2+                        |                     | 73 LS |       |     |
|             |                       |                           |                     | 80 HS |       |     |
|             |                       | 3+                        |                     | 61.5  |       |     |

\* CN = 3

**TABLE 4.6** Atom Radii and Effective Ionic Radii of Elements (*Continued*)

| Element                          | Atom radius, pm | Effective ionic radii, pm |                     |                  |        |     |
|----------------------------------|-----------------|---------------------------|---------------------|------------------|--------|-----|
|                                  |                 | Ion charge                | Coordination number |                  |        |     |
|                                  |                 |                           | 4                   | 6                | 8      | 12  |
| Chromium<br>( <i>continued</i> ) |                 | 4+                        | 41                  | 55               |        |     |
|                                  |                 | 5+                        | 34.5                | 49               | 57     |     |
|                                  |                 | 6+                        | 26                  | 44               |        |     |
| Cobalt                           | 125             | 2+                        | 38                  | 65 LS<br>74.5 HS | 90     |     |
|                                  |                 | 3+                        |                     | 54.5 LS<br>61 HS |        |     |
| Copper                           | 128             | 4+                        | 40                  | 53 HS            |        |     |
|                                  |                 | 1+                        | 60                  | 77               |        |     |
|                                  |                 | 2+                        | 57                  | 73               |        |     |
|                                  |                 | 3+                        |                     | 54 LS            |        |     |
| Curium                           | 174             | 3+                        |                     | 97               |        |     |
|                                  |                 | 4+                        |                     | 85               | 95     |     |
| Dysprosium                       | 178.1           | 2+                        |                     | 107              | 119    |     |
|                                  |                 | 3+                        |                     | 91.2             | 102.7  |     |
| Einsteinium                      | 186(2)          | 3+                        |                     | 98               |        |     |
| Erbium                           | 176.1           | 3+                        |                     | 89.0             | 100.4  |     |
| Europium                         | 208.4           | 2+                        |                     | 117              | 125    | 135 |
|                                  |                 | 3+                        |                     | 94.7             | 106.6  |     |
| Fluorine                         | 71.7            | 1−                        | 131                 | 133              |        |     |
|                                  |                 | 7+                        |                     | 8                |        |     |
| Francium                         | 270             | 1+                        |                     | 180              |        |     |
| Gadolinium                       | 180.4           | 3+                        |                     | 93.8             | 105.3  |     |
| Gallium                          | 135             | 2+                        |                     | 120              |        |     |
|                                  |                 | 3+                        | 47                  | 62.0             |        |     |
| Germanium                        | 128             | 2+                        |                     | 73               |        |     |
|                                  |                 | 4+                        | 39.0                | 53.0             |        |     |
| Gold                             | 144             | 1+                        |                     | 137              |        |     |
|                                  |                 | 3+                        | 68                  | 85               |        |     |
| Hafnium                          | 159             | 4+                        | 58                  | 71               | 83     |     |
| Holmium                          | 176.2           | 3+                        |                     | 90.1             | 101.5* | 112 |
| Hydrogen                         |                 | 1−                        |                     | 154              |        |     |
| Indium                           | 167             | 1+                        |                     | 140              |        |     |
|                                  |                 | 3+                        | 62                  | 80.0             | 92     |     |
| Iodine                           |                 | 1−                        |                     | 220              |        |     |
|                                  |                 | 5+                        |                     | 95               |        |     |
|                                  |                 | 7+                        | 42                  | 53               |        |     |
| Iridium                          | 135.5           | 3+                        |                     | 68               |        |     |
|                                  |                 | 4+                        |                     | 62.5             |        |     |
|                                  |                 | 5+                        |                     | 57               |        |     |
| Iron                             | 126             | 2+                        |                     | 61 LS            |        |     |
|                                  |                 |                           | 63 HS               | 78 HS            | 92 HS  |     |
|                                  |                 | 3+                        |                     | 55 LS            |        |     |
|                                  |                 |                           | 49 HS               | 64.5 HS          | 78 HS  |     |
|                                  |                 | 4+                        |                     | 58.5             |        |     |
|                                  |                 | 6+                        | 25                  |                  |        |     |
| Lanthanum                        | 183             | 3+                        |                     | 103.2            | 116.0  | 136 |

\* CN = 10



TABLE 4.6 Atom Radii and Effective Ionic Radii of Elements (Continued)

| Element    | Atom<br>radius,<br>pm | Effective ionic radii, pm |                     |         |       |     |
|------------|-----------------------|---------------------------|---------------------|---------|-------|-----|
|            |                       | Ion<br>charge             | Coordination number |         |       |     |
|            |                       |                           | 4                   | 6       | 8     | 12  |
| Lead       | 175                   | 2+                        | 98                  | 119     | 129   | 149 |
|            |                       | 4+                        |                     | 78      | 94    |     |
| Lithium    | 152                   | 1+                        | 59                  | 76      |       |     |
| Lutetium   | 173.8                 | 3+                        |                     | 86.1    | 97.7  |     |
| Magnesium  | 160                   | 2+                        | 57                  | 72.0    | 89    |     |
| Manganese  | 127                   | 2+                        | 66 HS               | 67 LS   | 96    |     |
|            |                       |                           |                     | 83 HS   |       |     |
|            |                       | 3+                        |                     | 58 LS   |       |     |
|            |                       |                           |                     | 64.5 HS |       |     |
|            |                       | 4+                        | 39                  | 53      |       |     |
|            |                       | 5+                        | 33                  |         |       | 127 |
|            |                       | 6+                        | 25.5                |         |       |     |
|            |                       | 7+                        | 25                  | 46      |       |     |
| Mercury    | 151                   | 1+                        | 111*                | 119     |       |     |
|            |                       | 2+                        | 96                  | 102     | 114   |     |
| Molybdenum | 139                   | 3+                        |                     | 69      |       |     |
|            |                       | 4+                        |                     | 65.0    |       |     |
|            |                       | 5+                        | 46                  | 61      |       |     |
|            |                       | 6+                        | 41                  | 59      | 73†   |     |
| Neodymium  | 181.4                 | 2+                        |                     |         | 129   |     |
|            |                       | 3+                        |                     | 98.3    | 110.9 | 127 |
| Neptunium  | 155                   | 2+                        |                     | 110     |       |     |
|            |                       | 3+                        |                     | 101     |       |     |
|            |                       | 4+                        |                     | 87      | 98    |     |
|            |                       | 5+                        |                     | 75      |       |     |
|            |                       | 6+                        |                     | 72      |       |     |
|            |                       | 7+                        |                     | 71      |       |     |
| Nickel     | 124                   | 2+                        | 55                  | 69.0    |       |     |
|            |                       | 3+                        |                     | 56 LS   |       |     |
|            |                       |                           |                     | 60 HS   |       |     |
|            |                       | 4+                        |                     | 48 LS   |       | 79  |
| Niobium    | 146                   | 3+                        |                     | 72      |       |     |
|            |                       | 4+                        |                     | 68      | 79    |     |
|            |                       | 5+                        | 48                  | 64      | 74    |     |
| Nitrogen   |                       | 3−                        | 146                 |         |       |     |
|            |                       | 1+                        | 25                  |         |       |     |
|            |                       | 3+                        |                     | 16      |       |     |
|            |                       | 5+                        |                     | 13      |       |     |
| Nobelium   |                       | 2+                        |                     | 110     |       |     |
| Osmium     | 135                   | 4+                        |                     | 63.0    |       |     |
|            |                       | 5+                        |                     | 57.5    |       | 142 |
|            |                       | 6+                        |                     | 54.5    |       |     |
|            |                       | 7+                        |                     | 52.5    |       |     |
|            |                       | 8+                        | 39                  |         |       |     |
| Oxygen     |                       | 2−                        | 138                 | 140     | 142   |     |
| Palladium  | 137                   | 2+                        | 64                  | 86      |       |     |
|            |                       | 3+                        |                     | 76      |       |     |
|            |                       | 4+                        |                     | 61.5    |       |     |

\* CN = 3  
† CN = 7

**TABLE 4.6** Atom Radii and Effective Ionic Radii of Elements (*Continued*)

| Element       | Atom<br>radius,<br>pm | Effective ionic radii, pm |                     |       |      |     |      |
|---------------|-----------------------|---------------------------|---------------------|-------|------|-----|------|
|               |                       | Ion<br>charge             | Coordination number |       |      |     |      |
|               |                       |                           | 4                   | 6     | 8    | 12  |      |
| Phosphorus    | 108                   | 3−                        | 17                  | 212   | 96   | 164 |      |
|               |                       | 3+                        |                     | 44    |      |     |      |
|               |                       | 5+                        |                     | 38    |      |     |      |
| Platinum      | 138.5                 | 2+                        |                     | 80    |      |     |      |
|               |                       | 4+                        | 17                  | 62.5  | 96   | 164 |      |
|               |                       | 5+                        |                     | 57    |      |     |      |
| Plutonium     | 159                   | 3+                        |                     | 100   |      |     |      |
|               |                       | 4+                        |                     | 86    |      |     |      |
|               |                       | 5+                        | 17                  | 74    | 108  | 170 |      |
|               |                       | 6+                        |                     | 71    |      |     |      |
| Polonium      | 164                   | 2−                        |                     | (230) |      |     |      |
|               |                       | 4+                        |                     | 94    |      |     |      |
|               |                       | 6+                        | 137                 | 67    | 151  | 164 |      |
| Potassium     | 232                   | 1+                        |                     | 138   |      |     |      |
| Praseodymium  | 182.4                 | 3+                        |                     | 99    |      |     |      |
|               |                       | 4+                        |                     | 85    | 96   | 170 |      |
| Promethium    | 183.4                 | 3+                        | 97                  | 109.3 |      |     |      |
| Protoactinium | 163                   | 3+                        | 104                 |       |      |     |      |
|               |                       | 4+                        | 38                  | 90    | 101  | 172 |      |
|               |                       | 5+                        |                     | 78    | 91   |     |      |
| Radium        | (220)                 | 2+                        |                     | 38    | 63   |     | 148  |
| Rhenium       | 137                   | 4+                        |                     |       | 58   |     |      |
|               |                       | 5+                        | 55                  |       |      |     |      |
|               |                       | 6+                        | 53                  |       |      |     |      |
|               |                       | 7+                        | 38                  | 66.5  | 161  | 172 |      |
| Rhodium       | 134                   | 3+                        |                     | 60    |      |     |      |
|               |                       | 4+                        |                     | 55    |      |     |      |
|               |                       | 5+                        |                     | 152   |      |     |      |
| Rubidium      | 248                   | 1+                        | 38                  | 68    | 127  | 124 |      |
| Ruthenium     | 134                   | 3+                        |                     | 62.0  |      |     |      |
|               |                       | 4+                        |                     | 56.5  |      |     |      |
|               |                       | 5+                        |                     | 36    | 68   |     |      |
|               |                       | 7+                        | 95.8                |       | 87.0 | 124 |      |
|               |                       | 8+                        |                     |       |      |     | 62.0 |
| Samarium      | 180.4                 | 2+                        |                     |       |      |     | 95.8 |
|               |                       | 3+                        |                     | 74.5  |      |     |      |
| Scandium      | 162                   | 3+                        | 26                  | 198   | 130  | 139 |      |
| Selenium      | 116                   | 2−                        |                     | 50    |      |     |      |
|               |                       | 4+                        |                     | 42    |      |     |      |
|               |                       | 6+                        |                     | 40.0  |      |     |      |
| Silicon       | 118                   | 4+                        | 100                 | 115   | 118  | 144 |      |
| Silver        | 144                   | 1+                        |                     | 79    |      |     |      |
|               |                       | 2+                        |                     | 94    |      |     |      |
|               |                       | 3+                        |                     | 67    |      |     |      |
|               |                       | 4+                        | 99                  | 75    | 126  | 139 |      |
| Sodium        | 186                   | 1+                        |                     | 102   |      |     |      |
| Strontium     | 215                   | 2+                        |                     | 118   |      |     |      |
| Sulfur        | 106                   | 2−                        |                     | 184   |      |     |      |
|               |                       | 4+                        | 12                  | 37    | 12   | 12  |      |
|               |                       | 6+                        |                     | 29    |      |     |      |
|               |                       | 3+                        |                     | 72    |      |     |      |
| Tantalum      | 146                   | 3+                        |                     |       |      |     |      |

**TABLE 4.6** Atom Radii and Effective Ionic Radii of Elements (*Continued*)

| Element                          | Atom<br>radius,<br>pm | Effective ionic radii, pm |                     |       |       |      |
|----------------------------------|-----------------------|---------------------------|---------------------|-------|-------|------|
|                                  |                       | Ion<br>charge             | Coordination number |       |       |      |
|                                  |                       |                           | 4                   | 6     | 8     | 12   |
| Tantalum<br>( <i>continued</i> ) | 136                   | 4+                        |                     | 68    |       |      |
| Technetium                       |                       | 5+                        |                     | 64    | 74    |      |
|                                  |                       | 4+                        |                     | 64.5  |       |      |
|                                  |                       | 5+                        |                     | 60    |       |      |
|                                  |                       | 7+                        | 37                  | 56    |       |      |
| Tellurium                        | 142                   | 2−                        |                     | 221   |       |      |
|                                  |                       | 4+                        | 66                  | 97    |       |      |
|                                  |                       | 6+                        | 43                  | 56    |       |      |
| Terbium                          | 177.3                 | 3+                        |                     | 92.3  | 104.0 |      |
|                                  |                       | 4+                        |                     | 76    | 88    |      |
| Thallium                         | 170                   | 1+                        |                     | 150   | 159   | 170  |
|                                  |                       | 3+                        | 75                  | 88.5  | 98    |      |
| Thorium                          | 179                   | 4+                        |                     | 94    | 105   | 121  |
| Thullium                         | 175.9                 | 2+                        |                     | 103   |       |      |
|                                  |                       | 3+                        |                     | 88.0  | 99.4  | 105* |
| Tin                              | 151                   | 2+                        |                     | 118   |       |      |
|                                  |                       | 4+                        | 55                  | 69.0  | 81    |      |
| Titanium                         | 147                   | 2+                        |                     | 86    |       |      |
|                                  |                       | 3+                        |                     | 67.0  |       |      |
|                                  |                       | 4+                        | 42                  | 60.5  | 74    |      |
| Tungsten                         | 139                   | 4+                        |                     | 66    |       |      |
|                                  |                       | 5+                        |                     | 62    |       |      |
|                                  |                       | 6+                        | 42                  | 60    |       |      |
| Uranium                          | 156                   | 3+                        |                     | 102.5 |       |      |
|                                  |                       | 4+                        |                     | 89    | 100   | 117  |
|                                  |                       | 5+                        |                     | 76    |       |      |
|                                  |                       | 6+                        | 52                  | 73    | 86    |      |
| Vanadium                         | 134                   | 2+                        |                     | 79    |       |      |
|                                  |                       | 3+                        |                     | 64.0  |       |      |
|                                  |                       | 4+                        |                     | 58    | 72    |      |
|                                  |                       | 5+                        | 35.5                | 54    |       |      |
| Xenon                            |                       | 8+                        | 40                  | 48    |       |      |
| Ytterbium                        | 193.3                 | 2+                        |                     | 102   | 114   |      |
|                                  |                       | 3+                        |                     | 86.8  | 98.5  | 104* |
| Yttrium                          | 180                   | 3+                        |                     | 90.0  | 101.9 | 108* |
| Zinc                             | 134                   | 2+                        | 60                  | 74.0  | 90    |      |
| Zirconium                        | 160                   | 4+                        | 59                  | 72    | 84    | 89*  |

\* CN = 11

4.5.2 Ionic Radii

One of the major factors in determining the structures of the substances that can be thought of as made up of cations and anions packed together is ionic size. It is obvious from the nature of wave functions that no ion has a precisely defined radius. However, with the insight afforded by electron

density maps and with a large base of data, new efforts to establish tables of ionic radii have been made, the most successful being those of Shannon and Prewitt. Pertinent references: R. D. Shannon and C. T. Prewitt, *Acta Crystallographica* **B25**:925 (1969); **B26**:1046 (1970) and R. D. Shannon, *Acta Crystallographica* **A32**:751 (1976).

Shannon and Prewitt base their *effective ionic radii* on the assumption that the ionic radius of  $O^{2-}$  (CN 6) is 140 pm and that of  $F^{-}$  (CN 6) is 133 pm. Also taken into consideration is the coordination number (CN) and electronic spin state (HS and LS, high spin and low spin) of first-row transition metal ions. These radii are empirical and include effects of covalence in specific metal-oxygen or metal-fluorine bonds. Older “crystal ionic radii” were based on the radius of  $F^{-}$  (CN 6) equal to 119 pm; these radii are 14–18 percent larger than the effective ionic radii.

### 4.5.3 Covalent Radii

Covalent radii (Table 4.7) are the distance between two kinds of atoms connected by a covalent bond of a given type (single, double, etc.).

**TABLE 4.7** Covalent Radii for Atoms

| Element    | Single-bond<br>radius, pm* | Double-bond<br>radius, pm | Triple-bond<br>radius, pm |
|------------|----------------------------|---------------------------|---------------------------|
| Aluminum   | 126                        |                           |                           |
| Antimony   | 141                        | 131                       |                           |
| Arsenic    | 121                        | 111                       |                           |
| Beryllium  | 106                        |                           |                           |
| Boron      | 88                         |                           |                           |
| Bromine    | 114                        | 104                       |                           |
| Cadmium    | 148                        |                           |                           |
| Carbon     | 77.2                       | 66.7                      | 60.3                      |
| Chlorine   | 99                         | 89                        |                           |
| Copper     | 135                        |                           |                           |
| Fluorine   | 64                         | 54                        |                           |
| Gallium    | 126                        |                           |                           |
| Germanium  | 122                        | 112                       |                           |
| Hydrogen   | 30                         |                           |                           |
| Indium     | 144                        |                           |                           |
| Iodine     | 133                        | 123                       |                           |
| Magnesium  | 140                        |                           |                           |
| Mercury    | 148                        |                           |                           |
| Nitrogen   | 70                         | 60                        | 55                        |
| Oxygen     | 66                         | 55                        |                           |
| Phosphorus | 110                        | 100                       | 93                        |
| Silicon    | 117                        | 107                       | 100                       |
| Selenium   | 117                        | 107                       |                           |
| Silver     | 152                        |                           |                           |
| Sulfur     | 104                        | 94                        | 87                        |
| Tellurium  | 137                        | 127                       |                           |
| Tin        | 140                        | 130                       |                           |
| Zinc       | 131                        |                           |                           |

\* Single-bond radii are for a tetrahedral (CN = 4) structure.

TABLE 4.8 Octahedral Covalent Radii for CN = 6

| Atom         | Octahedral<br>covalent<br>radius, pm | Atom          | Octahedral<br>covalent<br>radius, pm |
|--------------|--------------------------------------|---------------|--------------------------------------|
| Cobalt(II)   | 132                                  | Nickel(III)   | 130                                  |
| Cobalt(III)  | 122                                  | Nickel(IV)    | 121                                  |
| Gold(IV)     | 140                                  | Osmium(II)    | 133                                  |
| Iridium(III) | 132                                  | Palladium(IV) | 131                                  |
| Iron(II)     | 123                                  | Platinum(IV)  | 131                                  |
| Iron(IV)     | 120                                  | Rhodium(III)  | 132                                  |
| Nickel(II)   | 139                                  | Ruthenium(II) | 133                                  |

TABLE 4.9 Bond Lengths between Carbon and Other Elements

| Bond type                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |          | Bond length, pm |           |          |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|-----------|----------|
| Carbon-carbon                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |          |                 |           |          |
| Single bond<br>Paraffinic: —C—C—<br>In presence of —C=C— or of aromatic ring<br>In presence of —C=O bond<br>In presence of two carbon-oxygen bonds<br>In presence of two carbon-carbon double bonds<br>Aryl-C=O<br>In presence of one carbon-carbon triple bond: —C—C≡C—<br>In presence of one carbon-nitrogen triple bond: —C—C≡N<br>In compounds with tendency to dipole formation, e.g., C=C—C=O<br>In aromatic compounds<br>In presence of carbon-carbon double and triple bonds: —C=C—C≡C—<br>In presence of two carbon-carbon triple bonds: —C≡C—C≡C—<br>Double bond<br>Single: —C=C—<br>Conjugated with a carbon-carbon double bond: —C=C—C=C—<br>Conjugated with a carbon-oxygen double bond: —C=C—C=O<br>Cumulative: —C=C=C— or —C=C=O<br>Triple bond<br>Simple: —C≡C—<br>Conjugated: —C≡C—C=C—, —C≡C—C=O, or —C≡C—aryl |          | 154.1(3)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 153(1)          |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 151.6(5)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 149(1)          |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 142.6(5)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 147(2)          |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 146.0(3)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 146.6(5)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 144(1)          |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 139.5(3)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 142.6(5)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 137.3(4)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 133.7(6)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 133.6(5)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 136(1)          |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 130.9(5)        |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          |                 |           | 120.4(2) |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |          | 120.6(4)        |           |          |
| Bond type                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |          | Bond length, pm |           |          |
| Carbon-halogen                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |          |                 |           |          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Fluorine | Chlorine        | Bromine   | Iodine   |
| Paraffinic: R—X                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 137.9(5) | 176.7(2)        | 193.8(5)  | 213.9(1) |
| Olenfinic: —C=C—X                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 133.3(5) | 171.9(5)        | 189(1)    | 209.2(5) |
| Aromatic: Ar-X                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 132.8(5) | 170(1)          | 185(1)    | 205(1)   |
| Acetylenic: —C≡C—X                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | (127)    | 163.5(5)        | 179.5(10) | 199(2)   |

**TABLE 4.9** Bond Lengths between Carbon and Other Elements (*Continued*)

| Bond type                                                                                                         | Bond length, pm |
|-------------------------------------------------------------------------------------------------------------------|-----------------|
| Carbon-hydrogen                                                                                                   |                 |
| Paraffinic                                                                                                        |                 |
| In methane (in CD <sub>4</sub> , 109.2)                                                                           | 109.4           |
| In monosubstituted carbon: $\text{H}-\text{C}-\text{Y}$                                                           | 109.6(5)        |
| $\begin{array}{c} \text{X} \\   \\ \text{H}-\text{C}- \\   \\ \text{Y} \end{array}$                               |                 |
| In disubstituted carbon:                                                                                          | 107.3(5)        |
| $\begin{array}{c} \text{X} \\   \\ \text{H}-\text{C}- \\   \\ \text{Y} \end{array}$                               |                 |
| In trisubstituted carbon: $\text{H}-\text{C}-\text{Y}$                                                            | 107.0(7)        |
| $\begin{array}{c} \text{X} \\   \\ \text{H}-\text{C}-\text{Y} \\   \\ \text{Z} \end{array}$                       |                 |
| Olefinic                                                                                                          |                 |
| Simple: $\text{H}-\text{C}=\text{C}-$                                                                             | 108.3(5)        |
| Cumulative carbon-carbon double bonds: $\text{H}-\text{C}=\text{C}=\text{C}-$                                     | 107(1)          |
| Cumulative carbon-carbon-oxygen double bonds: $\text{H}-\text{C}-\text{C}=\text{C}=\text{O}$                      | 108(1)          |
| Aromatic                                                                                                          | 108.4(5)        |
| Acetylenic (in C <sub>2</sub> H <sub>2</sub> , 105.9)                                                             | 105.5(5)        |
| In small rings                                                                                                    | 108.1(5)        |
| In presence of a carbon triple bond: $\text{H}-\text{C}\equiv\text{C}-$                                           | 111.5(4)        |
| Carbon-nitrogen                                                                                                   |                 |
| Single bond                                                                                                       |                 |
| Paraffinic:                                                                                                       |                 |
| 3-covalent nitrogen: RNH <sub>2</sub> , R <sub>2</sub> NH, R <sub>3</sub> N                                       | 147.2(5)        |
| 4-covalent nitrogen: RNH <sub>3</sub> <sup>+</sup> , R <sub>3</sub> N-BX <sub>3</sub>                             | 147.9(5)        |
| In $-\text{C}-\text{N}=-$                                                                                         | 147.5(10)       |
| In aromatic compounds                                                                                             | 143(1)          |
| In conjugated heterocyclic systems (partial double bond)                                                          | 135.3(5)        |
| In $-\text{N}-\text{C}=\text{O}$ (partial double bond)                                                            | 132.2(5)        |
| Double bond: $-\text{C}=\text{N}-$                                                                                | 132             |
| Triple bond (in CN radical, 117.74): $-\text{C}\equiv\text{N}$                                                    | 115.7(5)        |
| Carbon-oxygen                                                                                                     |                 |
| Single bond                                                                                                       |                 |
| Paraffinic and saturated heterocyclic: $-\text{C}-\text{O}-$                                                      | 142.6(5)        |
| Strained, as in epoxides: $\begin{array}{c} \text{C}-\text{C} \\ \diagup \quad \diagdown \\ \text{O} \end{array}$ | 143.5(5)        |
| In aromatic compounds, as Ar-OH                                                                                   | 136(1)          |
| Longer bond in carboxylic acids and esters (HCOOH, 131.2)                                                         | 135.8(5)        |
| In conjugated heterocyclics, as furan                                                                             | 137.1(16)       |
| Double bond                                                                                                       |                 |
| In CO <sup>+</sup>                                                                                                | 111.5           |
| In CO                                                                                                             | 112.8           |
| In CO <sub>2</sub> <sup>+</sup>                                                                                   | 117.7           |
| In HCO                                                                                                            | 119.8(8)        |
| In carbonyls                                                                                                      | 114.5(10)       |
| In aldehydes and ketones                                                                                          | 121.5(5)        |

**TABLE 4.9** Bond Lengths between Carbon and Other Elements (*Continued*)

| Bond type                                                     |                 | Bond length, pm |                 |
|---------------------------------------------------------------|-----------------|-----------------|-----------------|
| Carbon-oxygen ( <i>continued</i> )                            |                 |                 |                 |
| In acyl halides: R—CO—X                                       |                 | 117.1(4)        |                 |
| Shorter bond in carboxylic acids and esters                   |                 | 123.3(5)        |                 |
| In zwitterion forms                                           |                 | 126(1)          |                 |
| In O=C=                                                       |                 | 116.0(1)        |                 |
| In isocyanates: RN=C=O                                        |                 | 117(1)          |                 |
| In conjugated systems, as in partial triple bond: O=C—C≡C     |                 | 121.5(5)        |                 |
| In 1,4-quinones                                               |                 | 115(2)          |                 |
| In metal acetylacetonates                                     |                 | 128(2)          |                 |
| In calcite: CaCO <sub>3</sub>                                 |                 | 129(1)          |                 |
| Carbon-selenium                                               |                 |                 |                 |
| Single bond                                                   |                 |                 |                 |
| Paraffinic: —C—Se—                                            |                 | 198(2)          |                 |
| In presence of fluorine, as in perfluorocompounds: —CF—Se—    |                 | 195(2)          |                 |
| Double bond                                                   |                 |                 |                 |
| In Se=C=, as SeCS and SeCO                                    |                 | 170.9(3)        |                 |
| In CSe radical                                                |                 | 167             |                 |
| Carbon-silicon                                                |                 |                 |                 |
| Alkyl substituent: H <sub>3</sub> C—Si or H <sub>2</sub> C—Si |                 | 187.0(5)        |                 |
| Aryl substituent: aryl—Si                                     |                 | 184.3(5)        |                 |
| Electronegative substituent: R—Si—X                           |                 | 185.4(5)        |                 |
| Carbon-sulfur                                                 |                 |                 |                 |
| Single bond                                                   |                 |                 |                 |
| Paraffinic: —C—S—                                             |                 | 181.7(5)        |                 |
| In presence of fluorine, as in perfluoro compounds: —CF—S—    |                 | 183.5(1)        |                 |
| In heterocyclic systems: partial double bonds                 |                 | 171.8(5)        |                 |
| Double bonds                                                  |                 |                 |                 |
| In S=C; thiophene, S=CR <sub>2</sub>                          |                 | 171(1)          |                 |
| In sulfoxides and sulfones                                    |                 | 180(1)          |                 |
| In presence of second carbon-carbon double bond: S=C—C=C—     |                 | 155.5(1)        |                 |
| In SC radical [in CS <sub>2</sub> <sup>+</sup> , 155.4(5)]    |                 | 153.49(2)       |                 |
| Bond type                                                     | Bond length, pm | Bond type       | Bond length, pm |
| Other elements and carbon                                     |                 |                 |                 |
| C-Al                                                          | 224(4)          | C-Cr            | 192(4)          |
| C-As                                                          | 198(1)          | C-Fe            | 184(2)          |
| C-B                                                           | 156(1)          | C-Ge            |                 |
| C-Be                                                          | 193             | Alkyl           | 193(3)          |
| C-Bi                                                          | 230             | Aryl            | 194.5(5)        |
| C-Co                                                          | 183(2)          |                 |                 |

**TABLE 4.9** Bond Lengths between Carbon and Other Elements (*Continued*)

| Bond type                                      | Bond length, pm | Bond type                   | Bond length, pm |
|------------------------------------------------|-----------------|-----------------------------|-----------------|
| Other elements and carbon ( <i>continued</i> ) |                 |                             |                 |
| C-Hg                                           | 207(1)          | C-Sn                        |                 |
| in Hg(CN) <sub>2</sub>                         | 199(2)          | Alkyl                       | 214.3(5)        |
| C-In                                           | 216(4)          | Electronegative substituent | 218(2)          |
| C-Mo                                           | 208(4)          | C-Te                        | 190.4           |
| C-Ni                                           | 210.7(5)        | C-Tl                        | 270.5(5)        |
| C-Pb (alkyl)                                   | 230(1)          | C-W                         | 206             |
| C-Pd                                           | 227(4)          |                             |                 |
| C-Sb (paraffinic)                              | 220.2(16)       |                             |                 |

**TABLE 4.10** Bond Lengths between Elements Other than Carbon

| Elements | Bond type                                | Bond length, pm | Elements | Bond type                            | Bond length, pm |
|----------|------------------------------------------|-----------------|----------|--------------------------------------|-----------------|
| Boron    |                                          |                 | Nitrogen |                                      |                 |
| B-B      | B <sub>2</sub> H <sub>6</sub>            | 177(1)          | N-Cl     | NO <sub>2</sub> Cl                   | 179(2)          |
| B-Br     | BBr <sub>3</sub>                         | 187(2)          | N-F      | NF <sub>3</sub>                      | 136(2)          |
| B-Cl     | BCl <sub>3</sub>                         | 172(1)          | N-H      | NH <sub>4</sub> <sup>+</sup>         | 103.4(3)        |
| B-F      | BF <sub>3</sub> , R <sub>2</sub> BF      | 129(1)          |          | NH <sub>3</sub> , RNH <sub>2</sub>   | 101.2           |
| B-H      | Boranes                                  | 121(2)          |          | H <sub>2</sub> NNH <sub>2</sub>      | 103.8           |
|          | Bridge                                   | 139(2)          |          | R—CO—NH <sub>2</sub>                 | 99(3)           |
| B-N      | Borazoles                                | 142(1)          |          | HN=C=S                               | 101.3(5)        |
| B-O      | B(OH) <sub>3</sub> , (RO) <sub>3</sub> B | 136(5)          | N-D      | ND (N <sup>2</sup> H)                | 104.1           |
| Hydrogen |                                          |                 | N-N      | HN <sub>3</sub>                      | 102(1)          |
| H-Al     | AlH                                      | 164.6           |          | R <sub>2</sub> NNH <sub>2</sub>      | 145.1(5)        |
| H-As     | AsH <sub>3</sub>                         | 151.9           |          | N <sub>2</sub> O                     | 112.6(2)        |
| H-Be     | BeH                                      | 134.3           |          | N <sub>2</sub> <sup>+</sup>          | 111.6           |
| H-Br     | HBr                                      | 140.8           | N-O      | NO <sub>2</sub> Cl                   | 124(1)          |
| H-Ca     | CaH                                      | 200.2           |          | RO—NO <sub>2</sub>                   | 136(2)          |
| H-Cl     | HCl                                      | 127.4           |          | NO <sub>2</sub>                      | 118.8(5)        |
| H-F      | HF                                       | 91.7            | N=O      | N <sub>2</sub> O                     | 118.6(2)        |
| H-Ge     | GeH <sub>4</sub>                         | 153             |          | RNO <sub>2</sub>                     | 122(1)          |
| H-I      | HI                                       | 160.9           |          | NO <sup>+</sup>                      | 106.19          |
| H-K      | KH                                       | 224.4           | N-Si     | SiN                                  | 157.2           |
| H-Li     | LiH                                      | 159.5           | Oxygen   |                                      |                 |
| H-Mg     | MgH                                      | 173.1           | O-H      | H <sub>2</sub> O                     | 95.8            |
| H-Na     | NaH                                      | 188.7           |          | ROH                                  | 97(1)           |
| H-Sb     | H <sub>3</sub> Sb                        | 170.7           |          | OH <sup>+</sup>                      | 102.89          |
| H-Se     | H <sub>2</sub> Se                        | 146.0           |          | HOOH                                 | 96.0(5)         |
| H-Sn     | SnH <sub>4</sub>                         | 170.1           |          | D <sub>2</sub> O (2H <sub>2</sub> O) | 95.75           |
| D-Br     | DBr (2HBr)                               | 141.44          |          | OD                                   | 96.99           |
| D-Cl     | DCl                                      | 127.46          | O-O      | HO—OH                                | 148(1)          |
| D-I      | DI                                       | 161.65          |          | O <sub>2</sub> <sup>+</sup>          | 122.7           |
| T-Br     | TBr (3HBr)                               | 141.44          |          | O <sub>2</sub> <sup>-</sup>          | 126(2)          |
| T-Cl     | TCl                                      | 127.40          |          | O <sub>2</sub> <sup>2-</sup>         | 149(2)          |

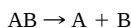


**TABLE 4.10** Bond Lengths between Elements Other than Carbon (*Continued*)

| Elements                    | Bond type                                      | Bond length, pm | Elements | Bond type                               | Bond length, pm |
|-----------------------------|------------------------------------------------|-----------------|----------|-----------------------------------------|-----------------|
| Oxygen ( <i>continued</i> ) |                                                |                 | Silicon  |                                         |                 |
| O-Al                        | O <sub>3</sub>                                 | 127.8(5)        | Si-Br    | SiBr <sub>4</sub> , R <sub>3</sub> SiBr | 216(1)          |
| O-As                        | AlO                                            | 161.8           | Si-Cl    | SiCl <sub>4</sub> , R <sub>3</sub> SiCl | 201.9(5)        |
| O-Ba                        | As <sub>2</sub> O <sub>6</sub> bridges         | 179             | Si-F     | SiF <sub>4</sub> , R <sub>3</sub> SiF   | 156.1(3)        |
| O-Cl                        | BaO                                            | 190.0           |          | SiF <sub>6</sub>                        | 158             |
|                             | ClO <sub>2</sub>                               | 148.4           | Si-H     | SiH <sub>4</sub>                        | 148.0(5)        |
|                             | OCl <sub>2</sub>                               | 168             |          | R <sub>3</sub> SiH                      | 147.6(5)        |
| O-Mg                        | MgO                                            | 174.9           | Si-I     | SiI <sub>4</sub>                        | 234             |
| O-Os                        | OsO <sub>4</sub>                               | 166             |          | R <sub>3</sub> SiI                      | 246(2)          |
| O-Pb                        | PbO                                            | 193.4           | Si-O     | R <sub>3</sub> SiOR                     | 153.3(5)        |
| Phosphorus                  |                                                |                 | Si-Si    | H <sub>3</sub> SiSiH <sub>3</sub>       | 230(2)          |
| P-Br                        | PBr <sub>3</sub>                               | 223(1)          | Sulfur   |                                         |                 |
| P-Cl                        | PCl <sub>3</sub>                               | 200(2)          | S-Br     | SOBr <sub>2</sub>                       | 227(2)          |
| P-F                         | PFCl <sub>2</sub>                              | 155(3)          | S-Cl     | S <sub>2</sub> Cl <sub>2</sub>          | 158.5(5)        |
| P-H                         | PH <sub>3</sub> , PH <sub>4</sub> <sup>+</sup> | 142.4(5)        | S-F      | SOF <sub>2</sub>                        | 158.5(5)        |
| P-I                         | PI <sub>3</sub>                                | 252(1)          | S-H      | H <sub>2</sub> S                        | 133.3           |
| P-N                         | Single bond                                    | 149.1           |          | RSH                                     | 132.9(5)        |
| P-O                         | Single bond                                    | 144.7           |          | D <sub>2</sub> S                        | 134.5           |
|                             | <i>p</i> <sup>3</sup> bonding                  | 167             | S-O      | SO <sub>2</sub>                         | 143.21          |
|                             | <i>sp</i> <sup>3</sup> bonding                 | 154(4)          |          | SOCl <sub>2</sub>                       | 145(2)          |
| P-S                         | <i>p</i> <sup>3</sup> bonding                  | 212(5)          | S-S      | RSSR                                    | 205(1)          |
|                             | <i>sp</i> <sup>3</sup> bonding                 | 208(2)          |          |                                         |                 |
|                             | In rings                                       | 220(3)          |          |                                         |                 |
| P-C                         | Single bond                                    | 156.2           |          |                                         |                 |
|                             | <i>p</i> <sup>3</sup> bonding                  | 187(2)          |          |                                         |                 |

**TABLE 4.11** Bond Dissociation Energies

The bond dissociation energy (enthalpy change) for a bond A—B which is broken through the reaction



is defined as the standard-state enthalpy change for the reaction at a specified temperature, here at 298 K. That is,

$$\Delta H_{298}^{\circ} = \Delta H_{298}^{\circ}(\text{A}) + \Delta H_{298}^{\circ}(\text{B}) - \Delta H_{298}^{\circ}(\text{AB})$$

All values refer to the gaseous state and are given at 298 K. Values of 0 K are obtained by subtracting  $\frac{3}{2}RT$  from the value at 298 K.

To convert the tabulated values to kcal/mol, divide by 4.184.

| Bond                  | $\Delta H_{298}^{\circ}$ ,<br>kJ/mol | Bond                          | $\Delta H_{298}^{\circ}$ ,<br>kJ/mol |
|-----------------------|--------------------------------------|-------------------------------|--------------------------------------|
| Aluminum              |                                      | Antimony ( <i>continued</i> ) |                                      |
| Al—Al                 | 186(9)                               | Sb—O                          | 372(84)                              |
| Al—As                 | 180                                  | Sb—P                          | 357                                  |
| Al—Au                 | 326(6)                               | Sb—S                          | 379                                  |
| Al—Br                 | 439(8)                               | Sb—Te                         | 277.4(38)                            |
| Al—C                  | 255                                  | Arsenic                       |                                      |
| Al—Cl                 | 494(13)                              | As—As                         | 382(11)                              |
| AlCl—Cl               | 402(8)                               | As—Cl                         | 448                                  |
| AlCl <sub>2</sub> —Cl | 372(8)                               | As—Ga                         | 209.6(12)                            |
| AlO—Cl                | 515(84)                              | As—H                          | 272(12)                              |
| Al—Cu                 | 216(10)                              | As—N                          | 582(126)                             |
| Al—D                  | 291                                  | As—O                          | 481(8)                               |
| Al—F                  | 664(6)                               | As—P                          | 534(13)                              |
| AlF—F                 | 546(42)                              | As—S                          | (478)                                |
| AlF <sub>2</sub> —F   | 544(46)                              | As—Se                         | 96                                   |
| AlO—F                 | 761(42)                              | As—Tl                         | 198(15)                              |
| Al—H                  | 285(6)                               | Astatine                      |                                      |
| Al—I                  | 368(4)                               | At—At                         | (115.9)                              |
| Al—Li                 | 176(15)                              | Barium                        |                                      |
| Al—N                  | 297(96)                              | Ba—Br                         | 370(8)                               |
| Al—O                  | 512(4)                               | Ba—Cl                         | 444(13)                              |
| AlCl—O                | 540(41)                              | Ba—F                          | 487(7)                               |
| AlF—O                 | 582                                  | Ba—I                          | > 431(4)                             |
| Al—P                  | 213(13)                              | Ba—O                          | 563(42)                              |
| Al—Pd                 | 259(12)                              | Ba—OH                         | 477(42)                              |
| Al—S                  | 374(8)                               | Ba—S                          | 400(19)                              |
| Al—Se                 | 334(10)                              | Beryllium                     |                                      |
| Al—Si                 | 251(3)                               | Be—Be                         | 59                                   |
| Al—Te                 | 268(10)                              | Be—Br                         | 381(84)                              |
| Al—U                  | 326(29)                              | Be—Cl                         | 388(9)                               |
| Antimony              |                                      |                               |                                      |
| Sb—Sb                 | 299(6)                               |                               |                                      |
| Sb—Br                 | 314(59)                              |                               |                                      |
| Sb—Cl                 | 360(50)                              |                               |                                      |
| Sb—F                  | 439(96)                              |                               |                                      |
| Sb—N                  | 301(50)                              |                               |                                      |

TABLE 4.11 Bond Dissociation Energies (Continued)

| Bond                             | $\Delta H_{298}^{\circ}$ ,<br>kJ/mol | Bond                                               | $\Delta H_{298}^{\circ}$ ,<br>kJ/mol |
|----------------------------------|--------------------------------------|----------------------------------------------------|--------------------------------------|
| Beryllium (continued)            |                                      | Bromine                                            |                                      |
| BeCl—Cl                          | 540(63)                              | Br—Br                                              | 193.870(4)                           |
| Be—F                             | 577(42)                              | Br—C                                               | 280(21)                              |
| Be—H                             | 226(21)                              | Br—CH <sub>3</sub>                                 | 284(8)                               |
| Be—O                             | 448(21)                              | Br—CH <sub>2</sub> Br                              | 255(13)                              |
| Be—S                             | 372(59)                              | Br—CHBr <sub>2</sub>                               | 259(17)                              |
| Bismuth                          |                                      | Br—CBr <sub>3</sub>                                | 209(13)                              |
| Bi—Bi                            | 197(4)                               | Br—CCl <sub>3</sub>                                | 218(13)                              |
| Bi—Br                            | 267(4)                               | Br—CF <sub>3</sub>                                 | 285(13)                              |
| Bi—Cl                            | 305(8)                               | Br—CF <sub>2</sub> CF <sub>3</sub>                 | 287.4(63)                            |
| Bi—D                             | 284                                  | Br—CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> | 278.2(63)                            |
| Bi—F                             | 259(29)                              | Br—CHF <sub>2</sub>                                | 289                                  |
| Bi—Ga                            | 159(17)                              | Br—Cl                                              | 218.84(4)                            |
| Bi—H                             | 279                                  | Br—CN                                              | 381                                  |
| Bi—O                             | 343(6)                               | Br—CO—C <sub>6</sub> H <sub>5</sub>                | 268                                  |
| Bi—P                             | 280(13)                              | Br—F                                               | 233.8(2)                             |
| Bi—Pb                            | 142(15)                              | Br—N                                               | 276(21)                              |
| Bi—S                             | 316(5)                               | Br—NF <sub>2</sub>                                 | 222                                  |
| Bi—Sb                            | 251(4)                               | Br—NO                                              | 120.1(63)                            |
| Bi—Se                            | 280(6)                               | Br—O                                               | 235.1(4)                             |
| Bi—Te                            | 232(11)                              | Cadmium                                            |                                      |
| Bi—Tl                            | 121(13)                              | Cd—Cd                                              | 11.3(8)                              |
| Boron                            |                                      | Cd—Br                                              | 159(96)                              |
| B—B                              | 297(21)                              | Cd—Cl                                              | 206.7(34)                            |
| H <sub>3</sub> B—BH <sub>3</sub> | 146                                  | Cd—F                                               | 305(21)                              |
| OB—BO                            | 506(84)                              | Cd—H                                               | 69.0(4)                              |
| B—Br                             | 435(21)                              | Cd—I                                               | 138(21)                              |
| B—C                              | 448(29)                              | Cd—In                                              | 138                                  |
| B—Cl                             | 536(29)                              | Cd—O                                               | 142(42)                              |
| BO—Cl                            | 460(42)                              | Cd—S                                               | 196                                  |
| B—D                              | 341(6)                               | Cd—Se                                              | 310                                  |
| B—F                              | 766(13)                              | Calcium                                            |                                      |
| BF—F                             | 523(63)                              | Ca—Ca                                              | 14.98(46)                            |
| BF <sub>2</sub> —F               | 557(84)                              | Ca—Br                                              | 321(23)                              |
| B—H                              | 330(4)                               | Ca—Cl                                              | 398(13)                              |
| B—I                              | 384(21)                              | Ca—F                                               | 527(21)                              |
| B—N                              | 389(21)                              | Ca—H                                               | 167.8                                |
| B—O                              | 806(5)                               | Ca—I                                               | 285(63)                              |
| BCl—O                            | 715(41)                              | Ca—O                                               | 464(84)                              |
| B—P                              | 347(17)                              | Ca—S                                               | 314(19)                              |
| B—S                              | 581(9)                               | Carbon                                             |                                      |
| B—Se                             | 462(15)                              | C—C                                                | 607(21)                              |
| B—Si                             | 289(29)                              | H <sub>3</sub> C—CH <sub>3</sub>                   | 368                                  |
| B—Te                             | 354(20)                              |                                                    |                                      |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

[illegible]

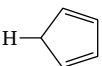
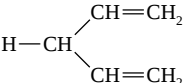
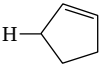
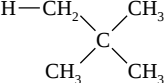
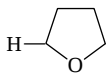
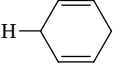
TABLE 4.11 Bond Dissociation Energies (Continued)

| Bond                                | $\Delta H_f^\circ_{298}$ ,<br>kJ/mol | Bond                 | $\Delta H_f^\circ_{298}$ ,<br>kJ/mol |
|-------------------------------------|--------------------------------------|----------------------|--------------------------------------|
| Cesium                              |                                      | Chromium (continued) |                                      |
| Cs—Cs                               | 41.75(93)                            | Cr—Cu                | 155(21)                              |
| Cs—Br                               | 397.5(42)                            | Cr—F                 | 437(20)                              |
| Cs—Cl                               | 439(21)                              | Cr—Ge                | 170(29)                              |
| Cs—F                                | 514(8)                               | Cr—H                 | 280(50)                              |
| Cs—H                                | 178.1(38)                            | Cr—I                 | 287(24)                              |
| Cs—I                                | 339(4)                               | Cr—N                 | 378(19)                              |
| Cs—O                                | 297(25)                              | Cr—O                 | 427(29)                              |
| Cs—OH                               | 385(13)                              | OCr—O                | 531(63)                              |
| Chlorine                            |                                      | O <sub>2</sub> Cr—O  | 477(84)                              |
|                                     |                                      | Cr—S                 | 339(21)                              |
| Cl—Cl                               | 242.580(16)                          | Cobalt               |                                      |
| Cl—C                                | 338(42)                              | Co—Co                | 167(25)                              |
| Cl—CH <sub>3</sub>                  | 339(21)                              | Co—Br                | 331(42)                              |
| Cl—CH <sub>3</sub> <sup>+</sup>     | 213                                  | Co—Cl                | 398(8)                               |
| Cl—C(CH <sub>3</sub> ) <sub>3</sub> | 328.4                                | Co—Cu                | 162(17)                              |
| Cl—CH <sub>2</sub> Cl               | 310(13)                              | Co—F                 | 435(63)                              |
| Cl—CCl <sub>3</sub>                 | 293(21)                              | Co—Ge                | 239(25)                              |
| Cl—CF <sub>3</sub>                  | 360(33)                              | Co—I                 | 235(81)                              |
| Cl—CCl <sub>2</sub> F               | 305(8)                               | Co—O                 | 368(21)                              |
| Cl—CClF <sub>2</sub>                | 318(8)                               | Co—S                 | 343(21)                              |
| Cl—CF <sub>2</sub> CF <sub>2</sub>  | 346.0(71)                            | Copper               |                                      |
| Cl—CH=CH <sub>2</sub>               | 351                                  | Cu—Cu                | 202(4)                               |
| Cl—CN                               | 439                                  | Cu—Br                | 331(25)                              |
| Cl—COCl                             | 328                                  | Cu—Cl                | 383(21)                              |
| Cl—COCH <sub>3</sub>                | 349.4                                | Cu—F                 | 431(13)                              |
| Cl—COC <sub>6</sub> H <sub>5</sub>  | 310(13)                              | Cu—Ga                | 216(15)                              |
| Cl—Cl <sup>+</sup>                  | 393                                  | Cu—Ge                | 209(21)                              |
| Cl—ClO                              | 143.3(42)                            | Cu—H                 | 280(8)                               |
| O <sub>3</sub> Cl—ClO <sub>4</sub>  | 243                                  | Cu—I                 | 197(21)                              |
| Cl—F                                | 250.54(8)                            | Cu—Ni                | 206(17)                              |
| O <sub>3</sub> Cl—F                 | 255                                  | Cu—O                 | 343(63)                              |
| Cl—N                                | 389(50)                              | Cu—S                 | 285(17)                              |
| Cl—NCl                              | 280                                  | Cu—Se                | 293(38)                              |
| Cl—NCl <sub>2</sub>                 | 381                                  | Cu—Sn                | 177(17)                              |
| Cl—NF <sub>2</sub>                  | ca. 134                              | Cu—Te                | 176(38)                              |
| Cl—NH <sub>2</sub>                  | 251(25)                              | Curium               |                                      |
| Cl—NO                               | 159(6)                               | Cm—O                 | 736                                  |
| Cl—NO <sub>2</sub>                  | 142(4)                               | Dysprosium           |                                      |
| Cl—O                                | 272(4)                               | Dy—F                 | 527(21)                              |
| OCl—O                               | 243(13)                              | Dy—O                 | 611(42)                              |
| O <sub>2</sub> Cl—O                 | 201(4)                               | Dy—Se                | 322(42)                              |
| Cl—P                                | 289(42)                              | Dy—Te                | 234(42)                              |
| Cl—SiCl <sub>3</sub>                | 464                                  |                      |                                      |
| Chromium                            |                                      |                      |                                      |
| Cr—Cr                               | 155(21)                              |                      |                                      |
| Cr—Br                               | 328(24)                              |                      |                                      |
| Cr—Cl                               | 366(24)                              |                      |                                      |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

| Bond                                               | $\Delta H_f^{\circ}_{298}$ ,<br>kJ/mol | Bond                         | $\Delta H_f^{\circ}_{298}$ ,<br>kJ/mol |
|----------------------------------------------------|----------------------------------------|------------------------------|----------------------------------------|
| Erbium                                             |                                        | Gallium ( <i>continued</i> ) |                                        |
| Er—F                                               | 565(17)                                | Ga—O                         | 285(63)                                |
| Er—O                                               | 611(13)                                | Ga—P                         | 230(13)                                |
| Er—S                                               | 418(42)                                | Ga—Sb                        | 209(13)                                |
| Er—Se                                              | 326(42)                                | Ga—Te                        | 251(25)                                |
| Er—Te                                              | 239(42)                                | Germanium                    |                                        |
| Europium                                           |                                        | Ge—Ge                        | 274(21)                                |
| Eu—Eu                                              | 33.5(165)                              | Ge—Br                        | 255(29)                                |
| Eu—Cl                                              | <i>ca.</i> 326                         | Ge—Cl                        | 431.8(4)                               |
| Eu—F                                               | 528(18)                                | Ge—F                         | 485(21)                                |
| Eu—O                                               | 557(13)                                | Ge—H                         | 321.3(8)                               |
| Eu—S                                               | 364(15)                                | Ge—O                         | 662(13)                                |
| Eu—Se                                              | 301(15)                                | Ge—S                         | 551.0(25)                              |
| Eu—Te                                              | 243(15)                                | Ge—Se                        | 490(21)                                |
| Fluorine                                           |                                        | Ge—Si                        | 301(21)                                |
| F—F                                                | 156.9(96)                              | Ge—Te                        | 402(8)                                 |
| F—F <sup>+</sup>                                   | >251                                   | Gold                         |                                        |
| F—CH <sub>3</sub>                                  | 452(21)                                | Au—Au                        | 221.3(21)                              |
| F—C(CH <sub>3</sub> ) <sub>3</sub>                 | 439                                    | Au—B                         | 368(11)                                |
| F—C <sub>6</sub> H <sub>5</sub>                    | 485                                    | Au—Be                        | 285(8)                                 |
| F—CCl <sub>3</sub>                                 | 444(21)                                | Au—Bi                        | 293(84)                                |
| F—CCl <sub>2</sub> F                               | 460(25)                                | Au—Cl                        | 343(10)                                |
| F—CClF <sub>2</sub>                                | 490(25)                                | Au—Co                        | 215(13)                                |
| F—CF <sub>3</sub>                                  | 523(17)                                | Au—Cr                        | 215(6)                                 |
| F—COCH <sub>3</sub>                                | 498                                    | Au—Cu                        | 232(9)                                 |
| F—FO                                               | 272(13)                                | Au—Fe                        | 187(17)                                |
| F—FO <sub>2</sub>                                  | 81.0                                   | Au—Ga                        | 294(15)                                |
| F—N                                                | 301(42)                                | Au—Ge                        | 277(15)                                |
| F—NF                                               | 318(25)                                | Au—H                         | 314(10)                                |
| F—NF <sub>2</sub>                                  | 243(8)                                 | Au—La                        | 80(5)                                  |
| F—NO                                               | 235.6(42)                              | Au—Li                        | 68.0(16)                               |
| F—NO <sub>2</sub>                                  | 197(25)                                | Au—Mg                        | 243(42)                                |
| Gadolinium                                         |                                        | Au—Mn                        | 185(13)                                |
| Gd—F                                               | 590(27)                                | Au—Ni                        | 274(21)                                |
| Gd—O                                               | 716(17)                                | Au—Pb                        | 130(42)                                |
| Gd—S                                               | 525(15)                                | Au—Pd                        | 143(21)                                |
| Gd—Se                                              | 431(15)                                | Au—Rh                        | 231(29)                                |
| Gallium                                            |                                        | Au—S                         | 418(25)                                |
| Ga—Ga                                              | 138(21)                                | Au—Si                        | 312(12)                                |
| Ga—Br                                              | 444(17)                                | Au—Sn                        | 244(17)                                |
| (CH <sub>3</sub> ) <sub>3</sub> Ga—CH <sub>3</sub> | 253                                    | Au—Te                        | 247(67)                                |
| Ga—Cl                                              | 481(13)                                | Au—U                         | 318(29)                                |
| Ga—F                                               | 577(15)                                | Hafnium                      |                                        |
| Ga—H                                               | <274                                   | Hf—C                         | 548(63)                                |
| Ga—I                                               | 339(10)                                | Hf—N                         | 534(29)                                |
|                                                    |                                        | Hf—O                         | 791(8)                                 |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

| Bond                                                                               | $\Delta H_{298}^\circ$ ,<br>kJ/mol | Bond                                                                               | $\Delta H_{298}^\circ$ ,<br>kJ/mol |
|------------------------------------------------------------------------------------|------------------------------------|------------------------------------------------------------------------------------|------------------------------------|
| Hydrogen                                                                           |                                    | Hydrogen ( <i>continued</i> )                                                      |                                    |
| H—H                                                                                | 436.002(4)                         | H—CHCl <sub>2</sub>                                                                | 414.2                              |
| H— <sup>2</sup> H or H—D                                                           | 439.446(4)                         | H—CCl <sub>3</sub>                                                                 | 377(8)                             |
| <sup>2</sup> H— <sup>2</sup> H or D—D                                              | 443.546(4)                         | H—CBr <sub>3</sub>                                                                 | 377(8)                             |
| H—Br                                                                               | 365.7(21)                          | H—CCl <sub>2</sub> CHCl <sub>2</sub>                                               | 393(8)                             |
| H—C                                                                                | 337.2(8)                           | H—CH <sub>2</sub> F                                                                | 423(8)                             |
| H—CH                                                                               | 452(33)                            | H—CHF <sub>2</sub>                                                                 | 423(8)                             |
| H—CH <sub>2</sub>                                                                  | 473(4)                             | H—CF <sub>3</sub>                                                                  | 444(13)                            |
| H—CH <sub>3</sub>                                                                  | 431(8)                             | H—CF <sub>2</sub> Cl                                                               | 435(4)                             |
| <sup>2</sup> H—C <sup>2</sup> H <sub>3</sub> or D—CD <sub>3</sub>                  | 442.75(25)                         | H—CH <sub>2</sub> CF <sub>3</sub>                                                  | 446(45)                            |
| H—C≡CH                                                                             | 523(4)                             | H—CF <sub>2</sub> CH <sub>3</sub>                                                  | 416(4)                             |
| H—CH=CH <sub>2</sub>                                                               | 427                                | H—CF <sub>2</sub> CF <sub>3</sub>                                                  | 431(63)                            |
| H—CH <sub>2</sub> CH <sub>3</sub>                                                  | 410(4)                             | H—CH <sub>2</sub> I                                                                | 431(8)                             |
| H—CH <sub>2</sub> C≡CH                                                             | 392.9(50)                          | H—CHI <sub>2</sub>                                                                 | 431(8)                             |
| H—CH <sub>2</sub> CH=CH <sub>2</sub>                                               | 356                                | H—CN                                                                               | 540(25)                            |
| H—cyclopropyl                                                                      | 423(13)                            | H—CH <sub>2</sub> CN                                                               | <i>ca.</i> 389                     |
| H—CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>                                  | 410(8)                             | H—CH(CH <sub>3</sub> )CN                                                           | 377(8)                             |
| H—CH(CH <sub>3</sub> ) <sub>2</sub>                                                | 395.4                              | H—C(CH <sub>3</sub> ) <sub>2</sub> CN                                              | 364(8)                             |
| H—cyclobutyl                                                                       | 397(13)                            | H—CH <sub>2</sub> NH <sub>2</sub>                                                  | 397(8)                             |
| H—CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>                                | 360                                | H—CH <sub>2</sub> Si(CH <sub>3</sub> ) <sub>3</sub>                                | 414(4)                             |
| H—CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>3</sub>                              | 397(4)                             | H—CH <sub>2</sub> COCH <sub>3</sub>                                                | 393(75)                            |
| H—C(CH <sub>3</sub> ) <sub>3</sub>                                                 | 381                                | H—Cl                                                                               | 431.8(4)                           |
|    | 339(4)                             | H—CO                                                                               | 126(8)                             |
|    | 335(4)                             | H—CHO                                                                              | 364(4)                             |
|   | 343(4)                             | H—COOH                                                                             | 377                                |
|  | 414(4)                             | H—COCH <sub>3</sub>                                                                | 364(4)                             |
| H—C(CH <sub>3</sub> ) <sub>2</sub> CH=CH <sub>2</sub>                              | 331                                | H—COCH <sub>2</sub> CH <sub>3</sub>                                                | 364(4)                             |
| H—cyclopentyl                                                                      | 395(42)                            |  | 385                                |
| H—CH <sub>2</sub> C(CH <sub>3</sub> ) <sub>3</sub>                                 | 418(4)                             | H—COC <sub>6</sub> H <sub>5</sub>                                                  | 364(4)                             |
| H—C <sub>6</sub> H <sub>5</sub>                                                    | 431                                | H—COCF <sub>3</sub>                                                                | 381(8)                             |
| H—CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>                                    | 356(4)                             | H—F                                                                                | 568.6(13)                          |
| H—C(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>                                   | 314                                | H—I                                                                                | 298.7(8)                           |
|  | 310                                | H—N                                                                                | 314(17)                            |
| H—cyclohexyl                                                                       | 399.6(42)                          | H—NH                                                                               | 377(8)                             |
| H—cycloheptyl                                                                      | 387.0(42)                          | H—NH <sub>2</sub>                                                                  | 435(8)                             |
| H—norbornyl                                                                        | 406(13)                            | H—NHCH <sub>3</sub>                                                                | 431(8)                             |
| H—CH <sub>2</sub> Br                                                               | 410(25)                            | H—N(CH <sub>3</sub> ) <sub>2</sub>                                                 | 397(8)                             |
| H—CHBr <sub>2</sub>                                                                | 435                                | H—NHC <sub>6</sub> H <sub>5</sub>                                                  | 335(13)                            |
| H—CH <sub>2</sub> Cl                                                               | 423                                | H—N(CH <sub>3</sub> )C <sub>6</sub> H <sub>5</sub>                                 | 310(13)                            |
|                                                                                    |                                    | HNF <sub>2</sub>                                                                   | 318(13)                            |
|                                                                                    |                                    | H—N <sub>3</sub>                                                                   | 356                                |
|                                                                                    |                                    | H—NO                                                                               | <205                               |
|                                                                                    |                                    | H—O                                                                                | 428.0(21)                          |
|                                                                                    |                                    | H—OH                                                                               | 498.7(8)                           |
|                                                                                    |                                    | H—OCH <sub>3</sub>                                                                 | 436.8(42)                          |
|                                                                                    |                                    | H—OCH <sub>2</sub> CH <sub>3</sub>                                                 | 436.0                              |
|                                                                                    |                                    | H—OC(CH <sub>3</sub> ) <sub>3</sub>                                                | 439(4)                             |
|                                                                                    |                                    | H—OC <sub>6</sub> H <sub>5</sub>                                                   | 368(25)                            |
|                                                                                    |                                    | H—ONO                                                                              | 327.6(25)                          |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

| Bond                                 | $\Delta H_{298}^\circ$ ,<br>kJ/mol | Bond                                               | $\Delta H_{298}^\circ$ ,<br>kJ/mol |
|--------------------------------------|------------------------------------|----------------------------------------------------|------------------------------------|
| Hydrogen ( <i>continued</i> )        |                                    | Iridium                                            |                                    |
| H—ONO <sub>2</sub>                   | 423.4(25)                          | Ir—O                                               | 352(21)                            |
| H—OOH                                | 374(8)                             | Ir—Si                                              | 463(21)                            |
| H—OOCCH <sub>3</sub>                 | 469(17)                            | Iron                                               |                                    |
| H—OOCCH <sub>2</sub> CH <sub>3</sub> | 460(17)                            | Fe—Fe                                              | 100(21)                            |
| H—OOCCH <sub>3</sub> H <sub>7</sub>  | 431(17)                            | Fe—Br                                              | 247(96)                            |
| H—P                                  | 343(29)                            | Fe—Cl                                              | ca. 352                            |
| H—S                                  | 344(12)                            | Fe—O                                               | 409(13)                            |
| H—SH                                 | 381(4)                             | Fe—S                                               | 339(21)                            |
| H—SCH <sub>3</sub>                   | ca. 368                            | Fe—Si                                              | 297(25)                            |
| H—Se                                 | 305(2)                             | Krypton                                            |                                    |
| H—Si                                 | 298.49(46)                         | Kr—Kr                                              | 5.4(8)                             |
| H—SiH <sub>3</sub>                   | 393(13)                            | Kr—F                                               | 54                                 |
| H—Si(CH <sub>3</sub> ) <sub>3</sub>  | 377(13)                            | Lanthanum                                          |                                    |
| H—Te                                 | 268(2)                             | La—La                                              | 247(21)                            |
| Indium                               |                                    | La—C                                               | 506(63)                            |
| In—In                                | 100(8)                             | La—F                                               | 598(42)                            |
| In—Br                                | 418(21)                            | La—N                                               | 519(42)                            |
| In—Cl                                | 439(8)                             | La—O                                               | 799(13)                            |
| In—F                                 | 506(15)                            | La—S                                               | 577(25)                            |
| In—O                                 | 360(21)                            | Lead                                               |                                    |
| In—P                                 | 197.9(85)                          | Pb—Pb                                              | 339(25)                            |
| In—S                                 | 289(17)                            | Pb—Br                                              | 247(38)                            |
| In—Sb                                | 152(11)                            | Pb(CH <sub>3</sub> ) <sub>3</sub> —CH <sub>3</sub> | 207(42)                            |
| In—Se                                | 247(17)                            | Pb—Cl                                              | 301(29)                            |
| In—Te                                | 218(17)                            | Pb—F                                               | 356(8)                             |
| Iodine                               |                                    | Pb—H                                               | 176(21)                            |
| I—I                                  | 152.549(8)                         | Pb—I                                               | 197(38)                            |
| I—Br                                 | 179.1(4)                           | Pb—O                                               | 378(4)                             |
| I—CH <sub>3</sub>                    | 232(13)                            | Pb—S                                               | 346.0(17)                          |
| I—C <sub>2</sub> H <sub>5</sub>      | 223.8                              | Pb—Se                                              | 303(4)                             |
| I—CH(CH <sub>3</sub> ) <sub>2</sub>  | 222                                | Pb—Te                                              | 251(13)                            |
| I—C(CH <sub>3</sub> ) <sub>3</sub>   | 207.1                              | Lithium                                            |                                    |
| I—CH <sub>2</sub> CF <sub>3</sub>    | 234(4)                             | Li—Li                                              | 106(4)                             |
| I—CF <sub>3</sub> CH <sub>3</sub>    | 216(4)                             | Li—Br                                              | 423(21)                            |
| I—C <sub>3</sub> F <sub>7</sub>      | 209(4)                             | Li—Cl                                              | 469(13)                            |
| I—CH=CHCH <sub>3</sub>               | 172                                | Li—F                                               | 577(21)                            |
| I—C <sub>6</sub> H <sub>5</sub>      | 268(4)                             | Li—H                                               | 247                                |
| I—C <sub>6</sub> F <sub>5</sub>      | 276                                | Li—I                                               | 352(13)                            |
| I—Cl                                 | 213.3(4)                           | Li—Na                                              | 88                                 |
| I—COCH <sub>3</sub>                  | 219.7                              | Li—O                                               | 341(6)                             |
| I—CN                                 | 305(4)                             | Li—OH                                              | 427(21)                            |
| I—F                                  | 280(4)                             |                                                    |                                    |
| I—N                                  | 159(17)                            |                                                    |                                    |
| I—NO                                 | 71(4)                              |                                                    |                                    |
| I—NO <sub>2</sub>                    | 75(4)                              |                                                    |                                    |
| I—O                                  | 184(21)                            |                                                    |                                    |



TABLE 4.11 Bond Dissociation Energies (Continued)

| Bond                                                           | $\Delta H_{298}^\circ$ ,<br>kJ/mol | Bond                | $\Delta H_{298}^\circ$ ,<br>kJ/mol |
|----------------------------------------------------------------|------------------------------------|---------------------|------------------------------------|
| Lutetium                                                       |                                    | Molybdenum          |                                    |
| Lu—Lu                                                          | 142(34)                            | Mo—I                | 372                                |
| Lu—F                                                           | 569(42)                            | Mo—O                | 607(34)                            |
| Lu—O                                                           | 695(13)                            | MoO—O               | 678(84)                            |
| Lu—S                                                           | 507(15)                            | MoO <sub>2</sub> —O | 565(84)                            |
| Lu—Te                                                          | 326(17)                            | Neodymium           |                                    |
| Magnesium                                                      |                                    | Nd—F                | 545(13)                            |
| Mg—Mg                                                          | 8.522(4)                           | Nd—O                | 703(34)                            |
| Mg—Br                                                          | 297(63)                            | Nd—S                | 474(15)                            |
| Mg—Cl                                                          | 318(13)                            | Nd—Se               | 385(17)                            |
| Mg—F                                                           | 462(21)                            | Nd—Te               | 305(17)                            |
| MgF—F                                                          | 569(42)                            | Neon                |                                    |
| Mg—H                                                           | 197(50)                            | Ne—Ne               | 3.93                               |
| Mg—I                                                           | ca. 285                            | Neptunium           |                                    |
| Mg—O                                                           | 394(35)                            | Np—O                | 720(29)                            |
| Mg—OH                                                          | 238(21)                            | Nickel              |                                    |
| Mg—S                                                           | 310(75)                            | Ni—Ni               | 261.9(25)                          |
| Manganese                                                      |                                    | Ni—Br               | 360(13)                            |
| Mn—Mn                                                          | 42(29)                             | Ni—Cl               | 372(21)                            |
| Mn—Br                                                          | 314(10)                            | Ni—F                | 435                                |
| Mn—Cl                                                          | 361(10)                            | Ni—H                | 289(13)                            |
| Mn—F                                                           | 423(15)                            | Ni—I                | 293(21)                            |
| Mn—I                                                           | 283(10)                            | Ni—O                | 391.6(38)                          |
| Mn—Cu                                                          | 159(17)                            | Ni—S                | 360(21)                            |
| Mn—O                                                           | 402(34)                            | Ni—Si               | 318(17)                            |
| Mn—S                                                           | 301(17)                            | Niobium             |                                    |
| Mn—Se                                                          | 201(13)                            | Nb—O                | 753(13)                            |
| Mercury                                                        |                                    | Nitrogen            |                                    |
| Hg—Hg                                                          | 17.2(21)                           | N—N                 | 945.33(59)                         |
| Hg—Br                                                          | 72.8(42)                           | N—Br                | 276(21)                            |
| CH <sub>3</sub> —HgCH <sub>3</sub>                             | 240.6                              | ON—Br               | 28.7(15)                           |
| C <sub>2</sub> H <sub>5</sub> —HgC <sub>2</sub> H <sub>5</sub> | 182.8(42)                          | N—Cl                | 389(50)                            |
| C <sub>3</sub> H <sub>7</sub> —HgC <sub>3</sub> H <sub>7</sub> | 197.1                              | ON—Cl               | 159(6)                             |
| Isopropyl—Hgisopropyl                                          | 170.3                              | O <sub>2</sub> N—Cl | 142(4)                             |
| C <sub>6</sub> H <sub>5</sub> —HgC <sub>6</sub> H <sub>5</sub> | 285                                | N—F                 | 301(42)                            |
| Hg—Cl                                                          | 100(8)                             | FN—F                | 318(21)                            |
| Hg—F                                                           | 130(38)                            | F <sub>2</sub> F—N  | 243(8)                             |
| Hg—H                                                           | 39.8                               | ON—F                | 236(4)                             |
| Hg—I                                                           | 38                                 | O <sub>2</sub> N—F  | 188(21)                            |
| Hg—K                                                           | 8.24(21)                           |                     |                                    |
| Hg—Na                                                          | >6.7                               |                     |                                    |
| Hg—S                                                           | 213                                |                     |                                    |
| Hg—Se                                                          | (167)                              |                     |                                    |
| Hg—Te                                                          | (142)                              |                     |                                    |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

| Bond                                              | $\Delta H_f^{\circ}_{298}$ ,<br>kJ/mol | Bond                                                           | $\Delta H_f^{\circ}_{298}$ ,<br>kJ/mol |         |
|---------------------------------------------------|----------------------------------------|----------------------------------------------------------------|----------------------------------------|---------|
| Nitrogen ( <i>continued</i> )                     |                                        | Oxygen ( <i>continued</i> )                                    |                                        |         |
| N—I                                               | 159(17)                                | C <sub>2</sub> H <sub>5</sub> O—OC <sub>2</sub> H <sub>5</sub> | 159                                    |         |
| F <sub>2</sub> N—NF <sub>2</sub>                  | 88(4)                                  | C <sub>3</sub> H <sub>7</sub> O—OC <sub>3</sub> H <sub>7</sub> | 155                                    |         |
| H <sub>2</sub> N—NH <sub>2</sub>                  | 297(8)                                 | Palladium                                                      |                                        |         |
| H <sub>2</sub> N—NHCH <sub>3</sub>                | 271                                    | Pd—O                                                           |                                        | 234(29) |
| H <sub>2</sub> N—N(CH <sub>3</sub> ) <sub>2</sub> | 264                                    | Phosphorus                                                     |                                        |         |
| H <sub>2</sub> N—NHC <sub>6</sub> H <sub>5</sub>  | 213                                    | P—P                                                            | 490(11)                                |         |
| HN—N <sub>2</sub>                                 | 38                                     | P—Br                                                           | 266.5                                  |         |
| ON—N                                              | 480.7(42)                              | P—C                                                            | 513(8)                                 |         |
| ON—NO <sub>2</sub>                                | 39.8(8)                                | P—Cl                                                           | 289(42)                                |         |
| O <sub>2</sub> N—NO <sub>2</sub>                  | 57.3(21)                               | P—F                                                            | 439(96)                                |         |
| HN=NH                                             | 456(42)                                | P—H                                                            | 343(29)                                |         |
| N≡N                                               | 946                                    | P—N                                                            | 617(21)                                |         |
| N—O                                               | 630.57(13)                             | P—O                                                            | 596.6                                  |         |
| HN=O                                              | 481                                    | Br <sub>3</sub> P=O                                            | 498(21)                                |         |
| NN—O                                              | 167                                    | Cl <sub>3</sub> P=O                                            | 510(21)                                |         |
| ON—O                                              | 305                                    | F <sub>3</sub> P=O                                             | 544(21)                                |         |
| N—P                                               | 617(21)                                | P—S                                                            | 346.0(17)                              |         |
| N—S                                               | 464(21)                                | P=S                                                            | 347                                    |         |
| Osmium                                            |                                        | P—Se                                                           | 363(10)                                |         |
| O <sub>3</sub> Os—O                               | 301(21)                                | P—Te                                                           | 298(10)                                |         |
| Oxygen                                            |                                        | Platinum                                                       |                                        |         |
| O—O                                               | 498.34(20)                             | Pt—B                                                           | 478(17)                                |         |
| O—Br                                              | 235.1(4)                               | Pt—H                                                           | 352(38)                                |         |
| HO—CH <sub>3</sub>                                | 377(13)                                | Pt—O                                                           | 347(34)                                |         |
| HO—CH=CH <sub>2</sub>                             | 364                                    | Pt—P                                                           | 417(17)                                |         |
| HO—CH <sub>2</sub> CH=CH <sub>2</sub>             | 456                                    | Pt—Si                                                          | 501(18)                                |         |
| HO—C <sub>6</sub> H <sub>5</sub>                  | 431                                    | Potassium                                                      |                                        |         |
| HO—CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>  | 322                                    | K—K                                                            | 57.3(42)                               |         |
| HO—CHO                                            | 402(13)                                | K—Br                                                           | 383(8)                                 |         |
| HO—COCH <sub>3</sub>                              | 452(21)                                | K—Cl                                                           | 427(8)                                 |         |
| HO—COC <sub>2</sub> H <sub>5</sub>                | 180                                    | K—F                                                            | 497.5(25)                              |         |
| O—Cl                                              | 272(4)                                 | K—H                                                            | 183(15)                                |         |
| HO—Cl                                             | 251(13)                                | K—I                                                            | 331(13)                                |         |
| O—F                                               | 222(17)                                | K—Na                                                           | 63.6(29)                               |         |
| O—FO                                              | 467                                    | K—O                                                            | 239(34)                                |         |
| FO—OF                                             | 261(84)                                | K—OH                                                           | 343(8)                                 |         |
| O—I                                               | 184(21)                                | Praseodymium                                                   |                                        |         |
| HO—I                                              | 234(13)                                | Pr—F                                                           | 582(46)                                |         |
| O—N                                               | 630.57(13)                             | Pr—O                                                           | 753(17)                                |         |
| HO—NCH <sub>3</sub>                               | 209                                    | Pr—S                                                           | 492.5(46)                              |         |
| HO—OC(CH <sub>3</sub> ) <sub>3</sub>              | 192(8)                                 |                                                                |                                        |         |
| HO—OH                                             | 213.8(21)                              |                                                                |                                        |         |
| O—OH                                              | 268(4)                                 |                                                                |                                        |         |
| CF <sub>3</sub> O—OCF <sub>3</sub>                | 192                                    |                                                                |                                        |         |
| CH <sub>3</sub> O—OCH <sub>3</sub>                | 157.3(8)                               |                                                                |                                        |         |

TABLE 4.11 Bond Dissociation Energies (Continued)

| Bond                     | $\Delta H_{298}^\circ$ ,<br>kJ/mol | Bond                                                                 | $\Delta H_{298}^\circ$ ,<br>kJ/mol |
|--------------------------|------------------------------------|----------------------------------------------------------------------|------------------------------------|
| Praseodymium (continued) |                                    | Scandium                                                             |                                    |
| Pr—Se                    | 446(23)                            | Sc—Sc                                                                | 163(21)                            |
| Pr—Te                    | 326(42)                            | Sc—Br                                                                | 444(63)                            |
| Promethium               |                                    | Sc—C                                                                 | 393(63)                            |
|                          |                                    | Sc—Cl                                                                | 318                                |
| Pm—F                     | 540(42)                            | Sc—F                                                                 | 589(13)                            |
| Pm—O                     | 674(63)                            | Sc—N                                                                 | 469(84)                            |
| Pm—S                     | 423(63)                            | Sc—O                                                                 | 674(13)                            |
| Pm—Se                    | 339(63)                            | Sc—S                                                                 | 478(13)                            |
| Pm—Te                    | 255(63)                            | Sc—Se                                                                | 385(17)                            |
|                          |                                    | Sc—Te                                                                | 289(17)                            |
| Radium                   |                                    | Selenium                                                             |                                    |
| Ra—Cl                    | 343(75)                            | Se—Se                                                                | 332.6(4)                           |
| Rhodium                  |                                    | Se—Br                                                                | 297(84)                            |
|                          |                                    | Se—C                                                                 | 582(96)                            |
| Rh—Rh                    | 285(21)                            | Se—Cl                                                                | 322                                |
| Rh—B                     | 476(21)                            | Se—F                                                                 | 339(42)                            |
| Rh—C                     | 583.7(63)                          | Se—H                                                                 | 305(2)                             |
| Rh—O                     | 377(63)                            | Se—N                                                                 | 381(63)                            |
| Rh—Si                    | 395(18)                            | Se—O                                                                 | 423(13)                            |
| Rh—Ti                    | 391(15)                            | Se—P                                                                 | 364(10)                            |
| Rubidium                 |                                    | Se—S                                                                 | 381(21)                            |
|                          |                                    | Se—Si                                                                | 531(25)                            |
| Rb—Rb                    | 45.6(21)                           | Se—Te                                                                | 268(8)                             |
| Rb—Br                    | 389(13)                            | Silicon                                                              |                                    |
| Rb—Cl                    | 448(21)                            | Si—Si                                                                | 327(10)                            |
| Rb—F                     | 494(21)                            | Si—Br                                                                | 343(50)                            |
| Rb—H                     | 167(21)                            | Si—C                                                                 | 435(21)                            |
| Rb—I                     | 335(13)                            | Si—Cl                                                                | 456(42)                            |
| Rb—O                     | 255(84)                            | Si—F                                                                 | 540(13)                            |
| Rb—OH                    | 351(8)                             | Si—H                                                                 | 298.49(46)                         |
| Ruthenium                |                                    | Si—I                                                                 | 339(84)                            |
|                          |                                    | Si—N                                                                 | 439(38)                            |
| Ru—O                     | 481(63)                            | Si—O                                                                 | 798(8)                             |
| O <sub>3</sub> Ru—O      | 439                                | Si—S                                                                 | 619(13)                            |
| Ru—Si                    | 397(21)                            | Si—Se                                                                | 531(25)                            |
| Ru—Th                    | 592(42)                            | H <sub>3</sub> Si—SiH <sub>3</sub>                                   | 339(17)                            |
| Samarium                 |                                    | (CH <sub>3</sub> ) <sub>3</sub> Si—Si(CH <sub>3</sub> ) <sub>3</sub> | 339                                |
|                          |                                    | (Aryl) <sub>3</sub> Si—Si(aryl) <sub>3</sub>                         | 368(31)                            |
| Sm—Cl                    | 423(13)                            | Si—Te                                                                | 506(38)                            |
| Sm—F                     | 531(18)                            | Silver                                                               |                                    |
| Sm—O                     | 619(13)                            | Ag—Ag                                                                | 163(8)                             |
| Sm—S                     | 389                                | Ag—Au                                                                | 203(9)                             |
| Sm—Se                    | 331(15)                            | Ag—Bi                                                                | 193(42)                            |
| Sm—Te                    | 272(15)                            |                                                                      |                                    |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

| Bond                        | $\Delta H_{298}^\circ$ ,<br>kJ/mol | Bond      | $\Delta H_{298}^\circ$ ,<br>kJ/mol |
|-----------------------------|------------------------------------|-----------|------------------------------------|
| Silver ( <i>continued</i> ) |                                    | Tantalum  |                                    |
| Ag—Br                       | 293(29)                            | Ta—N      | 611(84)                            |
| Ag—Cl                       | 341.4                              | Ta—O      | 805(13)                            |
| Ag—Cu                       | 176(8)                             | Tellurium |                                    |
| Ag—F                        | 354(16)                            | Te—B      | 354(20)                            |
| Ag—Ga                       | 180(15)                            | Te—H      | 268(2)                             |
| Ag—Ge                       | 175(21)                            | Te—I      | 193(42)                            |
| Ag—H                        | 226(8)                             | Te—O      | 391(8)                             |
| Ag—I                        | 234(29)                            | Te—P      | 298(10)                            |
| Ag—In                       | 176(17)                            | Te—S      | 339(21)                            |
| Ag—O                        | 213(84)                            | Te—Se     | 268(8)                             |
| Ag—Sn                       | 136(21)                            | Terbium   |                                    |
| Ag—Te                       | 293(96)                            | Tb—F      | 561(42)                            |
| Sodium                      |                                    | Tb—O      | 707(13)                            |
| Na—Na                       | 77.0                               | Tb—S      | 515(42)                            |
| Na—Br                       | 370(13)                            | Tb—Te     | 339(42)                            |
| Na—Cl                       | 410(8)                             | Thallium  |                                    |
| Na—F                        | 481(8)                             | Tl—Tl     | 63                                 |
| Na—H                        | 201(21)                            | Tl—Br     | 333.9(17)                          |
| Na—I                        | 301(8)                             | Tl—Cl     | 372.8(21)                          |
| Na—K                        | 63.6(29)                           | Tl—F      | 445(19)                            |
| Na—O                        | 257(17)                            | Tl—H      | 188(8)                             |
| Na—OH                       | 381(13)                            | Tl—I      | 272(8)                             |
| Na—Rb                       | 59(4)                              | Thorium   |                                    |
| Strontium                   |                                    | Th—Th     | 289                                |
| Sr—Br                       | 332(19)                            | Th—C      | 484(25)                            |
| Sr—Cl                       | 406(13)                            | Th—N      | 577.4(21)                          |
| Sr—F                        | 542(7)                             | Th—O      | 854(13)                            |
| Sr—H                        | 163(8)                             | Th—P      | 377                                |
| Sr—I                        | 263(42)                            | Thullium  |                                    |
| Sr—O                        | 454(15)                            | Tm—F      | 569(42)                            |
| Sr—OH                       | 381(42)                            | Tm—O      | 557(13)                            |
| Sr—S                        | 314(21)                            | Tm—S      | 368(42)                            |
| Sulfur                      |                                    | Tm—Se     | 276(42)                            |
| S—S                         | 429(6)                             | Tm—Te     | 276(42)                            |
| S—Cl                        | 255                                | Tin       |                                    |
| S—F                         | 343(5)                             | Sn—Sn     | 195(17)                            |
| O <sub>2</sub> S—F          | 71                                 | Sn—Br     | 339(4)                             |
| S—N                         | 464(21)                            |           |                                    |
| S—O                         | 521.70(13)                         |           |                                    |
| OS—O                        | 551.4(84)                          |           |                                    |
| O <sub>2</sub> S—O          | 348.1(42)                          |           |                                    |
| HS—SH                       | 272(21)                            |           |                                    |

TABLE 4.11 Bond Dissociation Energies (*Continued*)

| Bond                                                                           | $\Delta H_f^\circ_{298}$ ,<br>kJ/mol | Bond                                                          | $\Delta H_f^\circ_{298}$ ,<br>kJ/mol |
|--------------------------------------------------------------------------------|--------------------------------------|---------------------------------------------------------------|--------------------------------------|
| Tin ( <i>continued</i> )                                                       |                                      | Vanadium ( <i>continued</i> )                                 |                                      |
| BrSn—Br                                                                        | 326                                  | V—Cl                                                          | 477(63)                              |
| Br <sub>3</sub> Sn—Br                                                          | 272                                  | V—F                                                           | 590(63)                              |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> Sn—C <sub>2</sub> H <sub>5</sub> | <i>ca.</i> 238                       | V—N                                                           | 477(8)                               |
| Sn—Cl                                                                          | 406(13)                              | V—O                                                           | 644(21)                              |
| Sn—F                                                                           | 467(13)                              | V—S                                                           | 490(16)                              |
| Sn—H                                                                           | 267(17)                              | V—Se                                                          | 347(21)                              |
| Sn—I                                                                           | 234(42)                              | Xenon                                                         |                                      |
| Sn—O                                                                           | 548(21)                              | Xe—Xe                                                         | 6.53(30)                             |
| Sn—S                                                                           | 464(3)                               | Xe—F                                                          | 13.0(4)                              |
| Sn—Se                                                                          | 401.3(59)                            | Xe—O                                                          | 36.4                                 |
| Sn—Te                                                                          | 319.2(8)                             | Ytterbium                                                     |                                      |
| Titanium                                                                       |                                      | Yb—Cl                                                         | 322                                  |
| Ti—Ti                                                                          | 141(21)                              | Yb—F                                                          | 521(10)                              |
| Ti—Br                                                                          | 439                                  | Yb—H                                                          | 159(38)                              |
| Ti—C                                                                           | 435(25)                              | Yb—O                                                          | 397.9(63)                            |
| Ti—Cl                                                                          | 494                                  | Yb—S                                                          | 167                                  |
| Ti—F                                                                           | 569(34)                              | Yttrium                                                       |                                      |
| Ti—H                                                                           | <i>ca.</i> 159                       | Y—Y                                                           | 159(21)                              |
| Ti—I                                                                           | 310(42)                              | Y—Br                                                          | 485(84)                              |
| Ti—N                                                                           | 464                                  | Y—C                                                           | 418(63)                              |
| Ti—O                                                                           | 662(16)                              | Y—Cl                                                          | 527(42)                              |
| Ti—S                                                                           | 426(8)                               | Y—F                                                           | 605(21)                              |
| Ti—Se                                                                          | 381(42)                              | Y—N                                                           | 481(63)                              |
| Ti—Te                                                                          | 289(17)                              | Y—O                                                           | 715.1(30)                            |
| Tungsten                                                                       |                                      | Y—S                                                           | 528(11)                              |
| W—Cl                                                                           | 423(42)                              | Y—Se                                                          | 435(13)                              |
| W—F                                                                            | 548(63)                              | Y—Te                                                          | 339(13)                              |
| W—O                                                                            | 653(25)                              | Zinc                                                          |                                      |
| OW—O                                                                           | 632(84)                              | Zn—Zn                                                         | 29                                   |
| O <sub>2</sub> W—O                                                             | 598(42)                              | Zn—Br                                                         | 142(29)                              |
| W—P                                                                            | 305(4)                               | C <sub>2</sub> H <sub>5</sub> C—C <sub>2</sub> H <sub>5</sub> | <i>ca.</i> 201                       |
| Uranium                                                                        |                                      | Zn—Cl                                                         | 229(20)                              |
| U—O                                                                            | 761(17)                              | Zn—F                                                          | 368(63)                              |
| OU—O                                                                           | 678(59)                              | Zn—H                                                          | 85.8(21)                             |
| O <sub>2</sub> U—O                                                             | 644(88)                              | Zn—I                                                          | 138(29)                              |
| U—S                                                                            | 523(10)                              | Zn—O                                                          | 284.1                                |
| Vanadium                                                                       |                                      | Zn—S                                                          | 205(13)                              |
| V—V                                                                            | 242(21)                              | Zn—Se                                                         | 136(13)                              |
| V—Br                                                                           | 439(42)                              | Zn—Te                                                         | 205                                  |
| V—C                                                                            | 469(63)                              |                                                               |                                      |

**TABLE 4.11** Bond Dissociation Energies (*Continued*)

| Bond      | $\Delta H_{298}^\circ$ ,<br>kJ/mol | Bond                           | $\Delta H_{298}^\circ$ ,<br>kJ/mol |
|-----------|------------------------------------|--------------------------------|------------------------------------|
| Zirconium |                                    | Zirconium ( <i>continued</i> ) |                                    |
| Zr—C      | 561(25)                            | Zr—O                           | 760(8)                             |
| Zr—F      | 623(63)                            | Zr—S                           | 575(17)                            |
| Zr—N      | 565(25)                            |                                |                                    |

**Source:** T. L. Cottrell, *The Strengths of Chemical Bonds*, 2d ed., Butterworth, London, 1958; B. deB. Darwent, *National Standard Reference Data Series*, National Bureau of Standards, no. 31, Washington, 1970; S. W. Benson, *J. Chem. Educ.* **42**:502 (1965); and J. A. Kerr, *Chem. Rev.* **66**:465 (1966).

## 4.6 BOND AND GROUP DIPOLE MOMENTS

All bonds between equal atoms are given zero values. Because of their symmetry, methane and ethane molecules are nonpolar. The principle of bond moments thus requires that the CH<sub>3</sub> group moment equal one H—C moment. Hence the substitution of any aliphatic H by CH<sub>3</sub> does not alter the dipole moment, and all saturated hydrocarbons have zero moments as long as the tetrahedral angles are maintained.

**TABLE 4.12** Bond Dipole Moments

| Bond               | Moment, D* | Bond                               | Moment, D* |
|--------------------|------------|------------------------------------|------------|
| H—C                |            | C—N, aliphatic                     | 0.45       |
| Aliphatic          | 0.3        | C=N                                | 1.4        |
| Aromatic           | 0.0        | C≡N (nitrile)                      | 3.6        |
| C—C                | 0.0        | NC (isonitrile)                    | 3.0        |
| C≡C                | 0.0        | N—H                                | 1.31       |
| C—O                |            | N—O                                | 0.3        |
| Ether, aliphatic   | 0.74       | N=O                                | 2.0        |
| Alcohol, aliphatic | 0.7        | N (lone pair on sp <sup>3</sup> N) | 1.0        |
| C=O                |            | C—P, aliphatic                     | 0.8        |
| Aliphatic          | 2.4        | P—O                                | (0.3)      |
| Aromatic           | 2.65       | P=O                                | 2.7        |
| O—H                | 1.51       | P—S                                | 0.5        |
| C—S                | 0.9        | P=S                                | 2.9        |
| C=S                | 2.0        | B—C, aliphatic                     | 0.7        |
| S—H                | 0.65       | B—O                                | 0.25       |
| S—O                | (0.2)      | Se—C                               | 0.7        |
| S=O                |            | Si—C                               | 1.2        |
| Aliphatic          | 2.8        | Si—H                               | 1.0        |
| Aromatic           | 3.3        | Si—N                               | 1.55       |

\* To convert debye units D into coulomb-meters, multiply by  $3.33564 \times 10^{-30}$ .

TABLE 4.12 Bond Dipole Moments (Continued)

| Bond  | Moment, D* | Bond                        | Moment, D* |
|-------|------------|-----------------------------|------------|
| H—Sb  | −0.08      | Br—F                        | 1.3        |
| H—As  | −0.10      | Cl—F                        | 0.88       |
| H—P   | 0.36       | Li—C                        | 1.4        |
| H—I   | 0.38       | K—Cl                        | 10.6       |
| H—Br  | 0.78       | K—F                         | 7.3        |
| H—Cl  | 1.08       | Cs—Cl                       | 10.5       |
| H—F   | 1.94       | Cs—F                        | 7.9        |
| C—Te  | 0.6        | Dative (coordination) bonds |            |
| N—F   | 0.17       | N → B                       | 2.6        |
| P—I   | 0.3        | O → B                       | 3.6        |
| P—Br  | 0.36       | S → B                       | 3.8        |
| P—Cl  | 0.81       | P → B                       | 4.4        |
| As—I  | 0.78       | N → O                       | 4.3        |
| As—Br | 1.27       | P → O                       | 2.9        |
| As—Cl | 1.64       | S → O                       | 3.0        |
| As—F  | 2.03       | As → O                      | 4.2        |
| Sb—I  | 0.8        | Se → O                      | 3.1        |
| Sb—Br | 1.9        | Te → O                      | 2.3        |
| Sb—Cl | 2.6        | P → S                       | 3.1        |
| S—Cl  | 0.7        | P → Se                      | 3.2        |
| Cl—O  | 0.7        | Sb → S                      | 4.5        |
| I—Br  | 1.2        |                             |            |
| I—Cl  | 1          |                             |            |
| Br—Cl | 0.57       |                             |            |

\* To convert debye units D into coulomb-meters, multiply by  $3.33564 \times 10^{-30}$ .

The group moment always includes the C—X bond. When the group is attached to an aromatic system, the moment contains the contributions through resonance of those polar structures postulated as arising through charge shifts around the ring.

All values for bond and group dipole moments in Tables 4.12 and 4.13 were obtained in benzene solutions.

TABLE 4.13 Group Dipole Moments

| Group                              | Moment, D*   |               |
|------------------------------------|--------------|---------------|
|                                    | Aromatic C—X | Aliphatic C—X |
| C—CH <sub>3</sub>                  | 0.37         | 0.0           |
| C—C <sub>2</sub> H <sub>5</sub>    | 0.37         | 0.0           |
| C—C(CH <sub>3</sub> ) <sub>3</sub> | 0.5          | 0.0           |
| C—CH=CH <sub>2</sub>               | <0.4         | 0.6           |
| C—C≡CH                             | 0.7          | 0.9           |
| C—F                                | 1.47         | 1.79          |

\* To convert debye units D into coulomb-meters, multiply by  $3.33564 \times 10^{-30}$ .

**TABLE 4.13** Group Dipole Moments (*Continued*)

| Group                                             | Moment, D*   |               |
|---------------------------------------------------|--------------|---------------|
|                                                   | Aromatic C—X | Aliphatic C—X |
| C—Cl                                              | 1.59         | 1.87          |
| C—Br                                              | 1.57         | 1.82          |
| C—I                                               | 1.40         | 1.65          |
| C—CH <sub>2</sub> F                               | 1.77         |               |
| C—CF <sub>3</sub>                                 | 2.54         | 2.32          |
| C—CH <sub>2</sub> Cl                              | 1.85         | 1.95          |
| C—CHCl <sub>2</sub>                               | 2.04         | 1.94          |
| C—CCl <sub>3</sub>                                | 2.11         | 1.57          |
| C—CH <sub>2</sub> Br                              | 1.86         | 1.96          |
| C—C≡N                                             | 4.05         | 3.4           |
| C—NC                                              | 3.5          | 3.5           |
| C—CH <sub>2</sub> CN                              | 1.86         | 2.0           |
| C—C=O                                             | 2.65         | 2.4           |
| C—CHO                                             | 2.96         | 2.49          |
| C—COOH                                            | 1.64         | 1.63          |
| C—CO—CH <sub>3</sub>                              | 2.96         | 2.49          |
| C—CO—OCH <sub>3</sub>                             | 1.83         | 1.75          |
| C—CO—OC <sub>2</sub> H <sub>5</sub>               | 1.9          | 1.8           |
| C—OH                                              | 1.6          | 1.7           |
| C—OCH <sub>3</sub>                                | 1.28         | 1.28          |
| C—OCF <sub>3</sub>                                | 2.36         |               |
| C—OCOCH <sub>3</sub>                              | 1.69         |               |
| C—OC <sub>6</sub> H <sub>5</sub>                  | 1.16         | 1.16          |
| C—CH <sub>2</sub> OH                              | 1.58         | 1.68          |
| C—NH <sub>2</sub>                                 | 1.53         | 1.46          |
| C—NHCH <sub>3</sub>                               | 1.71         |               |
| C—N(CH <sub>3</sub> ) <sub>2</sub>                | 1.58         | 0.86          |
| C—NHCOCH <sub>3</sub>                             | 3.69         |               |
| C—N(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>  | (0.3)        | −0.3          |
| C—NCO                                             | 2.32         | 2.8           |
| C—N <sub>3</sub>                                  | 1.44         |               |
| C—NO                                              | 3.09         |               |
| C—NO <sub>2</sub>                                 | 4.01         | 2.70          |
| C—CH <sub>2</sub> NO <sub>2</sub>                 | 3.3          | 3.4           |
| C—SH                                              | 1.22         | 1.55          |
| C—SCH <sub>3</sub>                                | 1.34         | 1.40          |
| C—SCF <sub>3</sub>                                | 2.50         |               |
| C—SCN                                             | 3.59         | 3.6           |
| C—NCS                                             | 2.9          | 3.3           |
| C—SC <sub>6</sub> H <sub>5</sub>                  | 1.51         | 1.5           |
| C—SF <sub>5</sub>                                 | 3.4          |               |
| C—SOCF <sub>3</sub>                               | 3.88         |               |
| (C—) <sub>2</sub> SO <sub>2</sub>                 | 5.05         | 4.53          |
| (C—) <sub>2</sub> SO <sub>2</sub> CH <sub>3</sub> | 4.73         |               |
| (C—) <sub>2</sub> SO <sub>2</sub> CF <sub>3</sub> | 4.32         |               |
| C—SeH                                             | 1.08         |               |
| C—SeCH <sub>3</sub>                               | 1.31         | 1.32          |
| C—Si(CH <sub>3</sub> ) <sub>3</sub>               | 0.44         | 0.4           |

\* To convert debye units D into coulomb-meters, multiply by  $3.33564 \times 10^{-30}$ .



4.7 MOLECULAR GEOMETRY

TABLE 4.14 Spatial Orientation of Common Hybrid Bonds

On the assumption that the pairs of electrons in the valency shell of a bonded atom in a molecule are arranged in a definite way which depends on the number of electron pairs (coordination number), the geometrical arrangement or shape of molecules may be predicted. A multiple bond is regarded as equivalent to a single bond as far as molecular shape is concerned.

| Coordination Number | Orbitals Hybridized    | Geometrical Arrangement                                                                                                   | Minimum Radius Ratio |
|---------------------|------------------------|---------------------------------------------------------------------------------------------------------------------------|----------------------|
| 2                   | $sp$<br>$dp$           | Linear                                                                                                                    |                      |
|                     | $p^2$<br>$ds$<br>$d^2$ | Bent (angular)                                                                                                            |                      |
| 3                   | $sp^2$<br>$ds^2$       | Trigonal planar                                                                                                           | 0.155                |
|                     | $p^3$<br>$d^2p$        | Trigonal pyramidal                                                                                                        |                      |
|                     | $sp^2d$<br>$p^2d^2$    | Square planar                                                                                                             |                      |
| 4                   | $sp^3$<br>$d^3s$       | Tetrahedral                                                                                                               | 0.225                |
|                     | $d^4$                  | Tetragonal pyramidal                                                                                                      |                      |
| 5                   | $sp^3d$<br>$d^3sp$     | Trigonal bipyramidal                                                                                                      | 0.155                |
| 6                   | $d^2sp^3$              | Octahedral                                                                                                                | 0.414                |
|                     | $d^4sp$                | Trigonal prism                                                                                                            |                      |
| 7                   |                        | One atom above the face of an octahedron, which is distorted chiefly by separating the atoms at the corners of this face. | 0.592                |
| 8                   | $d^4sp^3$              | Square antiprism (dodecahedral)                                                                                           | 0.645                |
|                     |                        | Cube                                                                                                                      | 0.732                |
| 9                   |                        | Formed by adding atoms beyond each of the vertical faces of a right triangular prism.                                     | 0.732                |
| 12                  |                        | Cube-octahedron                                                                                                           | 1.000                |

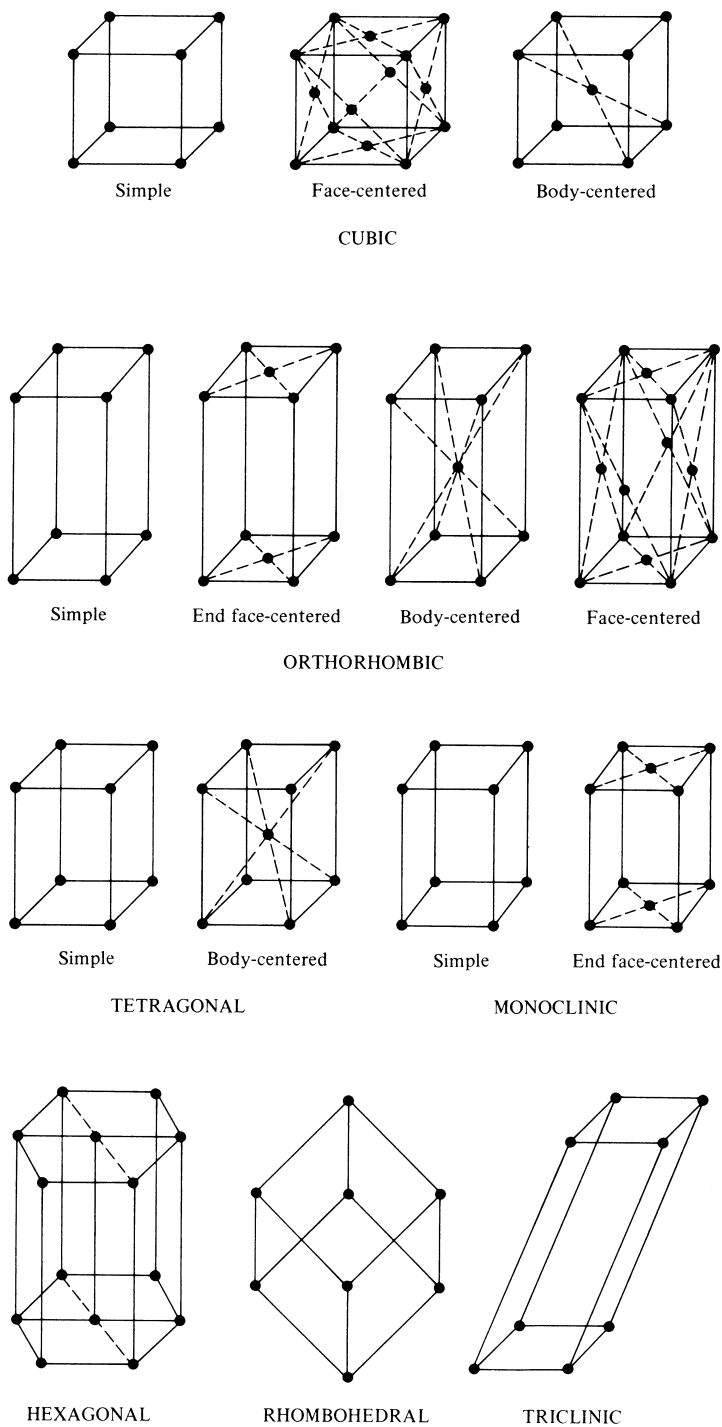


FIGURE 4.1 Crystal lattice types.

**TABLE 4.15** Crystal Structure

Unit cells of the different lattice types in each system are illustrated in Fig. 4.1.

| System                    | Characteristics                                                                                          | Essential Symmetry                                                                      | Axes in Unit Cell             | Angles in Unit Cell                                                                              |
|---------------------------|----------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|-------------------------------|--------------------------------------------------------------------------------------------------|
| Cubic                     | Three axes equal and mutually perpendicular                                                              | Four threefold axes                                                                     | $a = b = c$                   | $\alpha = \beta = \gamma = 90^\circ$                                                             |
| Tetragonal                | Two equal axes and one unequal axis mutually perpendicular                                               | One fourfold axis                                                                       | $a = b \neq c$                | $\alpha = \beta = \gamma = 90^\circ$                                                             |
| Orthorhombic (or rhombic) | Three unequal axes mutually perpendicular                                                                | Three mutually perpendicular twofold axes, or two planes intersecting in a twofold axis | $a \neq b \neq c$             | $\alpha = \beta = \gamma = 90^\circ$                                                             |
| Hexagonal or trigonal     | Three equal axes inclined at $120^\circ$ with a fourth axis unequal and perpendicular to the other three | One sixfold axis or one threefold axis                                                  | $a = b \neq c$<br>$a = b = c$ | $\alpha = \beta = 90^\circ$ ;<br>$\gamma = 120^\circ$<br>$\alpha = \beta = \gamma \neq 90^\circ$ |
| Monoclinic                | Two axes at an oblique angle with a third perpendicular to the other two                                 | One twofold axis or one plane                                                           | $a \neq b \neq c$             | $\alpha = \beta = 90^\circ$ ;<br>$\gamma \neq 90^\circ$                                          |
| Triclinic                 | Three unequal axes intersecting obliquely                                                                | No planes or axes of symmetry                                                           | $a \neq b \neq c$             | $\alpha \neq \beta \neq \gamma \neq 90^\circ$                                                    |
| Rhombohedral              | Two equal axes making equal angle with each other                                                        |                                                                                         |                               |                                                                                                  |

4.8 NUCLIDES

**TABLE 4.16** Table of Nuclides

Explanation of Column Headings

*Nuclide.* Each nuclide is identified by element name and the mass number  $A$ , equal to the sum of the numbers of protons  $Z$  and neutrons  $N$  in the nucleus. The  $m$  following the mass number (for example,  $^{69m}\text{Zn}$ ) indicates a metastable isotope. An asterisk preceding the mass number indicates that the radionuclide occurs in nature.

*Half-life.* The following abbreviations for time units are employed: y = years, d = days, h = hours, min = minutes, s = seconds, ms = milliseconds, and ns = nanoseconds.

*Natural abundance.* The natural abundances listed are on an “atom percent” basis for the stable nuclides present in naturally occurring elements in the earth’s crust.

*Thermal neutron absorption cross section.* Simply designated “cross section,” it represents the ease with which a given nuclide can absorb a thermal neutron (energy less than or equal to 0.025 eV) and become a different nuclide. The cross section is given here in units of barns (1 barn =  $10^{-24}$  cm<sup>2</sup>). If the mode of reaction is other than  $(n,\gamma)$ , it is so indicated.

*Major radiations.* In the last column are the principal modes of disintegration and energies of the radiations in million electronvolts (MeV). Symbols used to represent the various modes of decay are:

- $\alpha$ , alpha particle emission

$\beta^-$ , beta particle, negatron

$\beta^+$ , positron

$\gamma$ , gamma radiation
- K, electron capture

IT, isomeric transition

x, X-rays of indicated element (e.g., O-x, oxygen X-rays, and the type, K or L)

For  $\beta^-$  and  $\beta^+$ , values of  $E_{\text{max}}$  are listed. Radiation types and energies of minor importance are omitted unless useful for identification purposes. For detailed decay schemes the literature should be consulted.

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element    | A  | Half-life            | Natural abundance, % | Cross section, barns   | Radiation (MeV)                                          |
|------------|----|----------------------|----------------------|------------------------|----------------------------------------------------------|
| Hydrogen   | 1  |                      | 99.985(1)            | 0.332(2)               |                                                          |
|            | 2  |                      | 0.015(1)             | 0.000 52(1)            |                                                          |
|            | 3  | 12.32 y              |                      |                        | $\beta^-$ (0.0186)                                       |
| Beryllium  | 7  | 53.28 d              |                      |                        | K, $\gamma$ (0.478)                                      |
|            | 9  |                      | 100                  | 0.008(1)               |                                                          |
|            | 10 | $1.52 \times 10^6$ y |                      |                        | $\beta^-$ (0.555)                                        |
| Boron      | 10 |                      | 19.9(2)              | 3837(10)(n, $\alpha$ ) |                                                          |
|            | 11 |                      | 80.1(6)              | 0.005(3)               |                                                          |
| Carbon     | 11 | 20.3 min             |                      |                        | $\beta^+$ (0.961)                                        |
|            | 12 |                      | 98.89(1)             | 0.0035(1)              |                                                          |
|            | 14 | 5715 y               |                      |                        | $\beta^-$ (0.156)                                        |
| Nitrogen   | 13 | 9.965 min            |                      |                        | $\beta^+$ (1.190)                                        |
|            | 14 |                      | 99.634(9)            | 1.8(1)(n, p)           |                                                          |
| Oxygen     | 15 | 122.2 s              |                      |                        | $\beta^+$ (2.754)                                        |
|            | 19 | 26.9 s               |                      |                        | $\beta^-$ (4.82); $\gamma$ (0.197, 1.357)                |
| Fluorine   | 18 | 1.8295 h             |                      |                        | $\beta^+$ (0.635); K, O-x                                |
|            | 19 |                      | 100                  | 0.0095(7)              | $\beta^+$ (2.754)                                        |
|            | 20 | 11.00 s              |                      |                        | $\beta^-$ (5.40); $\gamma$ (1.63)                        |
| Sodium     | 22 | 2.605 y              |                      | 2800.(300)(n, p)       | $\beta^+$ (0.545, 1.83); K, Ne-x, $\gamma$ (1.275)       |
|            | 23 |                      | 100                  | 0.53                   |                                                          |
|            | 24 | 14.659 h             |                      |                        | $\beta^-$ (1.39); $\gamma$ (2.75, 1.37)                  |
| Magnesium  | 24 |                      | 78.89(3)             | 0.053(6)               |                                                          |
|            | 25 |                      | 10.00(1)             | 0.17(5)                |                                                          |
|            | 27 | 9.45 min             |                      | 0.07(2)                | $\beta^-$ (1.75, 1.59); $\gamma$ (0.844, 1.014)          |
|            | 28 | 20.90 h              |                      |                        | $\beta^-$ (0.459); $\gamma$ (1.342, 0.942, 0.401, 0.031) |
| Aluminum   | 26 | $7.1 \times 10^5$ y  |                      |                        | $\beta^+$ (1.16); K, Mg-x; $\gamma$ (1.809)              |
|            | 27 |                      | 100                  | 0.230(2)               |                                                          |
|            | 28 | 2.25 min             |                      |                        | $\beta^-$ (2.865); $\gamma$ (1.778)                      |
| Silicon    | 28 |                      | 92.23(2)             | 0.17(1)                |                                                          |
|            | 29 |                      | 4.67(2)              | 0.12(1)                |                                                          |
|            | 30 |                      | 3.10(1)              | 0.107(4)               |                                                          |
|            | 31 | 2.62 h               |                      | 0.073(6)               | $\beta^-$ (1.471); $\gamma$ (1.266)                      |
|            | 32 | $1.6 \times 10^2$ y  |                      |                        | $\beta^-$ (0.213)                                        |
| Phosphorus | 30 | 2.50 min             |                      |                        | $\beta^+$ (3.245)                                        |
|            | 31 |                      | 100                  | 0.16(2)                |                                                          |
|            | 32 | 14.28 d              |                      |                        | $\beta^-$ (1.710)                                        |
|            | 33 | 25.3 d               |                      |                        | $\beta^-$ (0.249)                                        |
| Sulfur     | 32 |                      | 95.02(9)             | 0.55(2)                |                                                          |
|            | 34 |                      | 4.21(8)              | 0.29(6)                |                                                          |
|            | 35 | 87.51 d              |                      |                        | $\beta^-$ (0.167)                                        |
|            | 37 | 5.05 min             |                      |                        | $\beta^-$ (4.75, 1.64); $\gamma$ (3.103, 0.908)          |
|            | 38 | 2.84 h               |                      |                        | $\beta^-$ (1.00, 3.0); $\gamma$ (1.942, 0.196)           |

TABLE 4.16 Table of Nuclides (Continued)

| Element   | A   | Half-life            | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                            |
|-----------|-----|----------------------|----------------------|----------------------|----------------------------------------------------------------------------|
| Chlorine  | 35  |                      | 75.77(5)             | 43.7(4)              |                                                                            |
|           | 36  | $3.01 \times 10^5$ y |                      | 46.(2)               | $\beta^-$ (0.709); K, S-x                                                  |
|           | 37  |                      | 24.23(5)             | 0.4                  |                                                                            |
|           | 38  | 37.24 min            |                      |                      | $\beta^-$ (4.91, 1.11, 2.77); $\gamma$ (2.168, 1.642)                      |
|           | 39  | 55.6 min             |                      |                      | $\beta^-$ (1.91, 2.18, 3.45); $\gamma$ (1.267, 0.250, 1.52)                |
| Argon     | 37  | 35.0 d               |                      |                      | K, Cl-x                                                                    |
|           | 39  | 268 y                |                      |                      | $\beta^-$ (0.565)                                                          |
|           | 40  |                      | 99.600(3)            | 0.64(3)              |                                                                            |
|           | 41  | 1.82 h               |                      | 0.5(1)               | $\beta^-$ (1.20, 2.49); $\gamma$ (1.29)                                    |
|           | 42  | 33 y                 |                      |                      | $\beta^-$ (0.60)                                                           |
| Potassium | 39  |                      | 93.258(4)            | 2.1(2)               |                                                                            |
|           | *40 | $1.26 \times 10^9$ y | 0.0117(1)            | 30.(8)               | $\beta^-$ (1.312); K, Ar-x; $\gamma$ (1.461)                               |
|           | 41  |                      | 6.730(4)             | 1.46(3)              |                                                                            |
|           | 42  | 12.360 h             |                      |                      | $\beta^-$ (3.523, 1.97); $\gamma$ (1.525)                                  |
|           | 43  | 22.3 h               |                      |                      | $\beta^-$ (0.825, 0.45, 1.24, 1.814); $\gamma$ (0.618, 0.373, 0.39, 0.221) |
|           |     |                      |                      |                      |                                                                            |
| Calcium   | 40  |                      | 96.941(18)           | 0.41(3)              |                                                                            |
|           | 42  | $1.02 \times 10^5$ y |                      | $\approx 4$          |                                                                            |
|           | 43  |                      | 0.135(6)             | 6.(1)                |                                                                            |
|           | 44  |                      | 2.086(12)            | 0.8(2)               |                                                                            |
|           | 45  | 162.7 d              |                      | $\approx 15$         | $\beta^-$ (0.257)                                                          |
|           | 47  | 4.536 d              |                      |                      | $\beta^-$ (1.98, 0.684); $\gamma$ (1.297)                                  |
|           | 49  | 8.72 min             |                      |                      | $\beta^-$ (1.95, 0.89); $\gamma$ (3.084, 4.07)                             |
|           |     |                      |                      |                      |                                                                            |
| Scandium  | 42m | 61.6 s               |                      |                      | $\beta^+$ (2.82); $\gamma$ (0.438, 1.227, 1.524)                           |
|           | 43  | 3.89 h               |                      |                      | $\beta^+$ (1.22)                                                           |
|           | 44m | 2.442 d              |                      |                      | IT, Sc-x; $\gamma$ (0.271)                                                 |
|           | 44  | 3.927 h              |                      |                      | $\beta^+$ (1.47); K, $\gamma$ (1.16)                                       |
|           | 45  |                      | 100                  | 27                   |                                                                            |
|           | 46m | 19.5 s               |                      |                      | $\gamma$ (0.142)                                                           |
|           | 46  | 83.81 d              |                      | 8.(1)                | $\beta^-$ (0.357); $\gamma$ (1.12, 0.889); Ti-x                            |
|           | 47  | 3.341 d              |                      |                      | $\beta^-$ (0.439, 0.60); $\gamma$ (0.159)                                  |
|           | 48  | 1.821 d              |                      |                      | $\beta^-$ (0.65); $\gamma$ (1.31, 1.04, 0.984)                             |
| Titanium  | 44  | 47.3 y               |                      |                      | K, $\gamma$ (0.68, 0.078)                                                  |
|           | 45  | 3.08 h               |                      |                      | $\beta^+$ (1.044); K, Sc-x                                                 |
|           | 48  |                      | 73.72(3)             | 7.9(9)               |                                                                            |
|           | 49  |                      | 5.41(2)              | 1.9(5)               |                                                                            |
|           | 50  |                      | 5.18(2)              | 0.179(3)             |                                                                            |
|           | 51  | 5.76 min             |                      |                      | $\beta^-$ (2.14, 1.50); $\gamma$ (0.320, 0.928)                            |
|           |     |                      |                      |                      |                                                                            |
| Vanadium  | 48  | 16.0 d               |                      |                      | $\beta^+$ (0.698); $\gamma$ (0.511, 0.945, 0.983, 1.312, 2.24)             |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                      | A      | Half-life               | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                                 |
|------------------------------|--------|-------------------------|----------------------|----------------------|---------------------------------------------------------------------------------|
| Vanadium<br>( <i>cont.</i> ) | 49     | 330 d                   |                      |                      | K, Ti-x                                                                         |
|                              | 50     | $>1.4 \times 10^{17}$ y | 0.250(2)             | 40.(20)              |                                                                                 |
|                              | 51     |                         | 99.750(2)            | 4.9(1)               |                                                                                 |
|                              | 52     | 3.75 min                |                      |                      | $\beta^-$ (2.47); $\gamma$ (1.434)                                              |
| Chromium                     | 48     | 21.6 h                  |                      |                      | K, V-x; $\gamma$ (0.116, 0.305)                                                 |
|                              | 50     |                         | 4.345(13)            | 15.(1)               |                                                                                 |
|                              | 51     | 27.70 d                 |                      |                      | K, V-x; $\gamma$ (0.320)                                                        |
|                              | 52     |                         | 83.79(2)             | 0.8(1)               |                                                                                 |
|                              | 53     |                         | 9.50(2)              | 18.(2)               |                                                                                 |
| Manganese                    | 51     | 46.2 min                |                      |                      | $\beta^+$ (2.2); $\gamma$ (0.749, 1.15)                                         |
|                              | 52     | 5.60 d                  |                      |                      | $\beta^+$ (0.575); $\gamma$ (0.511, 0.744, 1.434)                               |
|                              | 53     | $3.7 \times 10^6$ y     |                      | 70.(10)              |                                                                                 |
|                              | 54     | 312.2 d                 |                      | $<10$                | $\gamma$ (0.834)                                                                |
|                              | 55     |                         | 100                  | 13.3(1)              |                                                                                 |
|                              | 56     | 2.5785 h                |                      |                      | $\beta^-$ (1.028, 1.03, 0.718); $\gamma$ (0.847, 1.81, 2.11)                    |
| Iron                         | 52     | 8.275 h                 |                      |                      | $\beta^+$ (0.804); K, Mn-x; $\gamma$ (0.169)                                    |
|                              | 54     |                         | 5.85(4)              | 2.7(5)               |                                                                                 |
|                              | 55     | 2.73 y                  |                      | 13.(2)               | K, Mn-x                                                                         |
|                              | 56     |                         | 91.75(4)             | 2.6(2)               |                                                                                 |
|                              | 57     |                         | 2.12(1)              | 2.5(5)               |                                                                                 |
|                              | 59     | 44.51 d                 |                      | 13.(3)               | $\beta^-$ (0.273, 0.475); $\gamma$ (1.10, 1.29)                                 |
| Cobalt                       | 55     | 17.53 h                 |                      |                      | $\beta^+$ (1.04, 1.50); K, Fe-x; $\gamma$ (0.932, 0.480, 1.41)                  |
|                              | 56     | 77.3 d                  |                      |                      | $\beta^+$ (1.46); K, Fe-x; $\gamma$ (0.847, 1.04, 1.24, 1.77, 2.60, 3.26, 2.02) |
|                              | 57     | 271.77 d                |                      |                      | K, Fe-x; $\gamma$ (0.136, 0.122)                                                |
|                              | 58 $m$ | 9.1 h                   |                      | $1.4(1) \times 10^5$ | $\gamma$ (0.025)                                                                |
|                              | 58     | 70.88 d                 |                      | $1.9(2) \times 10^3$ | K, $\beta^+$ (0.474); Fe-x; $\gamma$ (0.811)                                    |
|                              | 59     |                         | 100                  | 19                   |                                                                                 |
|                              | 60 $m$ | 10.47 min               |                      | 58.(8)               | $\beta^-$ (1.55)                                                                |
|                              | 60     | 5.271 y                 |                      | 2.0(2)               | $\beta^-$ (0.318); $\gamma$ (1.173, 1.332)                                      |
|                              | 61     | 1.650 h                 |                      |                      | $\beta^-$ (1.22); $\gamma$ (0.842–0.909)                                        |
|                              |        |                         |                      |                      |                                                                                 |
| Nickel                       | 56     | 6.08 d                  |                      |                      | K, Co-x; $\gamma$ (0.158, 0.270, 0.480, 0.75, 0.812, 1.56)                      |
|                              | 57     | 35.6 h                  |                      |                      | K, $\beta^+$ (0.849, 0.712); Co-x, $\gamma$ (1.378, 0.0127, 1.76)               |
|                              | 58     |                         | 68.077(9)            | 4.6(4)               |                                                                                 |
|                              | 60     |                         | 26.22(1)             | 2.9(3)               |                                                                                 |
|                              | 63     | 100 y                   |                      | 24.(3)               | $\beta^-$ (0.067)                                                               |

TABLE 4.16 Table of Nuclides (Continued)

| Element                 | A      | Half-life | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                 |
|-------------------------|--------|-----------|----------------------|----------------------|-----------------------------------------------------------------|
| Nickel ( <i>cont.</i> ) | 64     |           | 0.926(1)             | 1.8(1)               |                                                                 |
|                         | 65     | 2.517 h   |                      | 22.(2)               | $\beta^-$ (2.14, 0.65, 1.020); $\gamma$ (1.48, 0.366, 1.116)    |
|                         | 66     | 2.275 d   |                      |                      | $\beta^-$ (0.23)                                                |
| Copper                  | 61     | 3.408 h   |                      |                      | $\beta^+$ (1.220); K, Ni-x; $\gamma$ (0.283, 0.656)             |
|                         | 63     |           | 69.17(3)             | 4.5(2)               |                                                                 |
|                         | 64     | 12.701 h  |                      | $\approx 270$        | $\beta^-$ (0.578); $\beta^+$ (0.65); Ni-x; $\gamma$ (1.346)     |
|                         | 65     |           | 30.83(3)             | 2.17(3)              |                                                                 |
|                         | 66     | 5.07 min  |                      | $1.4(1) \times 10^2$ | $\beta^-$ (2.74); $\gamma$ (1.039)                              |
|                         | 67     | 2.580 d   |                      |                      | $\beta^-$ (0.395, 0.484, 0.577); $\gamma$ (0.185, 0.092)        |
| Zinc                    | 62     | 9.26 h    |                      |                      | K, $\beta^+$ (0.66); Cu-x; $\gamma$ (0.041, 0.597)              |
|                         | 64     |           | 48.6(3)              | 0.46                 |                                                                 |
|                         | 65     | 243.8 d   |                      | 66.(8)               | K, $\beta^+$ (0.325), Cu-x; $\gamma$ (1.116)                    |
|                         | 66     |           | 27.9(2)              | 1.0(2)               |                                                                 |
|                         | 67     |           | 4.1(1)               | 6.9(1)               |                                                                 |
|                         | 68     |           | 18.8(4)              | 0.87                 |                                                                 |
|                         | 69 $m$ | 13.76 h   |                      |                      | IT, Zn-x, $\gamma$ (0.439)                                      |
|                         | 69     | 56 min    |                      |                      | $\beta^-$ (0.905)                                               |
|                         | 71 $m$ | 3.97 h    |                      |                      | $\beta^-$ (1.45); $\gamma$ (0.386, 0.487, 0.620)                |
|                         | 72     | 46.5 h    |                      |                      | $\beta^-$ (0.30, 0.25); $\gamma$ (0.145, 0.191)                 |
| Gallium                 | 66     | 9.5 h     |                      |                      | $\beta^+$ (1.84, 4.153); $\gamma$ (1.039, 2.752)                |
|                         | 67     | 3.260 d   |                      |                      | K, Zn-x; $\gamma$ (0.093, 0.184, 0.300)                         |
|                         | 68     | 1.130 h   |                      |                      | $\beta^+$ (1.83); K, Zn-x; $\gamma$ (1.077)                     |
|                         | 69     |           | 60.108(9)            | 1.68(7)              |                                                                 |
|                         | 70     | 21.1 min  |                      |                      | $\beta^-$ (1.65); $\gamma$ (0.175, 1.042)                       |
|                         | 71     |           | 39.892(9)            | 4.7(2)               |                                                                 |
|                         | 72     | 14.10 h   |                      |                      | $\beta^-$ (0.64, 1.51, 2.52, 3.15); $\gamma$ (0.63, 2.20, 2.50) |
|                         | 73     | 3.120 d   |                      |                      | $\beta^-$ (1.59); $\gamma$ (0.053, 0.297)                       |
| Germanium               | 66     | 2.66 h    |                      |                      | K, $\beta^+$ (1.02); Ga-x; $\gamma$ (0.044, 0.382)              |
|                         | 68     | 270.8 d   |                      |                      | Ga, K-x                                                         |
|                         | 69     | 1.63 d    |                      |                      | $\beta^+$ (0.70, 1.22); $\gamma$ (1.107, 0.574)                 |
|                         | 71     | 11.2 d    |                      |                      | Ga-x                                                            |
|                         | 72     |           | 27.66(3)             | 0.9(2)               |                                                                 |
|                         | 73     |           | 7.73(1)              | 15.(1)               |                                                                 |
|                         | 74     |           | 35.94(2)             | 0.3                  |                                                                 |
|                         | 75     | 1.380 h   |                      |                      | $\beta^-$ (1.19); $\gamma$ (0.265, 0.419)                       |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                       | A   | Half-life            | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                            |
|-------------------------------|-----|----------------------|----------------------|----------------------|----------------------------------------------------------------------------|
| Germanium<br>( <i>cont.</i> ) | 77  | 11.30 h              |                      |                      | $\beta^-$ (0.71, 1.38, 2.19);<br>$\gamma$ (0.211, 0.215, 0.264)            |
|                               | 78  | 1.45 h               |                      |                      | $\beta^-$ (0.95); $\gamma$ (0.277, 0.294)                                  |
| Arsenic                       | 71  | 2.70 d               |                      |                      | K, $\beta^+$ (0.81); Ge-x;<br>$\gamma$ (0.175, 1.096)                      |
|                               | 72  | 1.083 d              |                      |                      | $\beta^+$ (3.339, 2.498, 1.884);<br>K, Ge-x; $\gamma$ (0.834, 1.051)       |
|                               | 73  | 80.30 d              |                      |                      | K, $\gamma$ (0.0534, 0.0133)                                               |
|                               | 74  | 17.78 d              |                      |                      | $\beta^+$ (0.94); $\beta^-$ (0.71, 1.35);<br>$\gamma$ (0.596, 0.635)       |
|                               | 75  |                      | 100                  | 4.0(4)               |                                                                            |
|                               | 76  | 1.096 d              |                      |                      | $\beta^-$ (2.97, 2.41, 1.79);<br>$\gamma$ (0.559, 0.657)                   |
|                               | 77  | 38.8 h               |                      |                      | $\beta^-$ (0.683); $\gamma$ (0.239, 0.250, 0.521)                          |
|                               | 78  | 91 min               |                      |                      | $\beta^-$ (4.21); $\gamma$ (0.614, 0.70, 1.31)                             |
|                               | 79  |                      |                      |                      |                                                                            |
| Selenium                      | 72  | 8.40 d               |                      |                      | K, As-x; $\gamma$ (0.046)                                                  |
|                               | 73  | 7.1 h                |                      |                      | $\beta^+$ (1.32); $\gamma$ (0.361, 0.067)                                  |
|                               | 74  |                      | 0.89(2)              | 50.(4)               |                                                                            |
|                               | 75  | 119.78 d             |                      |                      | K, $\gamma$ (0.265, 0.136); As-x                                           |
|                               | 77m | 17.5 s               |                      |                      | $\gamma$ (0.162)                                                           |
|                               | 77  |                      | 7.63(6)              | 42.(4)               |                                                                            |
|                               | 80  |                      | 49.61(10)            | 0.5                  |                                                                            |
|                               | 81  | 18.5 min             |                      |                      | $\beta^-$ (1.58); $\gamma$ (0.276, 0.290, 0.828)                           |
| Bromine                       | 75  | 1.62 h               |                      |                      | $\beta^+$ (3.03); $\gamma$ (0.287)                                         |
|                               | 76  | 16.2 h               |                      | 224.(42)             | $\beta^+$ (1.9, 3.68); K, Se-x;<br>$\gamma$ (0.559, 1.86)                  |
|                               | 77  | 2.376 d              |                      |                      | $\gamma$ (0.239, 0.521)                                                    |
|                               | 79  |                      | 50.69(7)             | 10.8                 |                                                                            |
|                               | 80m | 4.42 h               |                      |                      | IT, Br-x; $\gamma$ (0.037, 0.049)                                          |
|                               | 80  | 17.66 min            |                      |                      | $\beta^-$ (1.997, 1.38); K,<br>$\beta^+$ (0.85), Se-x;<br>$\gamma$ (0.617) |
|                               | 81  |                      | 49.31(7)             | 2.6                  |                                                                            |
|                               | 82  | 1.4708 d             |                      |                      | $\beta^-$ (0.444); $\gamma$ (0.554, 0.619, 0.776)                          |
|                               | 83  |                      |                      |                      |                                                                            |
| Krypton                       | 76  | 14.8 h               |                      |                      | K, $\gamma$ (0.252)                                                        |
|                               | 77  | 1.24 h               |                      |                      | $\beta^+$ (1.875, 1.700, 1.550);<br>K, Br-x; $\gamma$ (0.130, 0.147)       |
|                               | 79  | 1.455 d              |                      |                      | $\beta^+$ (1.626); $\gamma$ (0.261, 0.398, 0.606)                          |
|                               | 81m | 13 s                 |                      |                      | IT, Kr-x; $\gamma$ (0.190)                                                 |
|                               | 81  | $2.10 \times 10^5$ y |                      |                      | K, Br-x; $\gamma$ (0.276)                                                  |
|                               | 83  |                      | 11.5(1)              | 183.(30)             |                                                                            |
|                               | 84  |                      | 57.0(3)              | 0.10                 |                                                                            |
|                               | 85m | 4.48 h               |                      |                      | $\beta^-$ (0.83); $\gamma$ (0.151, 0.305)                                  |
|                               | 86  |                      |                      |                      |                                                                            |



TABLE 4.16 Table of Nuclides (Continued)

| Element            | A   | Half-life               | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                |
|--------------------|-----|-------------------------|----------------------|----------------------|----------------------------------------------------------------|
| Krypton<br>(cont.) | 85  | 10.72 y                 |                      |                      | $\beta^-$ (0.67); $\gamma$ (0.517)                             |
|                    | 87  | 1.27 h                  |                      |                      | $\beta^-$ (3.49, 0.389, 1.38); $\gamma$ (0.403, 2.55)          |
|                    | 88  | 2.84 h                  |                      |                      | $\beta^-$ (2.91); $\gamma$ (0.196, 2.392)                      |
| Rubidium           | 84  | 32.9 d                  |                      |                      | $\beta^-$ (0.894); $\beta^+$ (2.681); $\gamma$ (0.882)         |
|                    | 85  |                         | 72.17(2)             | 0.5                  |                                                                |
|                    | 86  | 18.65 d                 |                      | < 20                 | $\beta^-$ (1.775); $\gamma$ (1.08)                             |
|                    | 87  | $4.88 \times 10^{10}$ y | 27.83(2)             | 0.10(1)              | $\beta^-$ (0.283)                                              |
|                    | 88  | 17.7 min                |                      | 1.2(3)               | $\beta^-$ (5.31); $\gamma$ (1.836, 0.898)                      |
|                    | 89  | 15.4 min                |                      |                      | $\beta^-$ (1.26, 2.2, 4.49); $\gamma$ (1.032, 1.248, 2.196)    |
| Strontium          | 82  | 25.36 d                 |                      |                      | K, Rb-x                                                        |
|                    | 85m | 1.126 h                 |                      |                      | K, Rb-x, Sr-x; $\gamma$ (0.150, 0.231)                         |
|                    | 85  | 64.84 d                 |                      |                      | K, Rb-x; $\gamma$ (0.514)                                      |
|                    | 87m | 2.795 h                 |                      |                      | IT, $\gamma$ (0.388)                                           |
|                    | 88  |                         | 82.58(1)             | 0.0058(4)            |                                                                |
|                    | 89  | 50.52 d                 |                      | 0.42(4)              | $\beta^-$ (1.497); $\gamma$ (0.909)                            |
|                    | 90  | 29.1 y                  |                      | 0.0097(7)            | $\beta^-$ (0.546)                                              |
|                    | 91  | 9.5 h                   |                      |                      | $\beta^-$ (1.09, 1.36, 2.66); $\gamma$ (0.556, 0.750, 1.024)   |
| Yttrium            | 92  | 2.71 h                  |                      |                      | $\beta^-$ (0.55, 1.5); $\gamma$ (1.383)                        |
|                    | 85m | 4.86 h                  |                      |                      | $\beta^+$ (2.24); K, Sr-x; $\gamma$ (0.767, 0.232, 2.124)      |
|                    | 85  | 2.68 h                  |                      |                      | $\beta^+$ (1.58, 1.15); K, Sr-x; $\gamma$ (0.504, 0.232)       |
|                    | 86  | 14.74 h                 |                      |                      | $\beta^+$ (5.24); $\gamma$ (0.307, 0.628, 1.077, 1.153, 1.921) |
|                    | 87m | 12.9 h                  |                      |                      | Y-x; $\gamma$ (0.381)                                          |
|                    | 88  | 106.6 d                 |                      |                      | $\beta^-$ (0.76); $\gamma$ (0.898, 1.836, 2.734, 3.219)        |
|                    | 90  | 2.67 d                  |                      | < 7                  | $\beta^-$ (2.28); $\gamma$ (2.186)                             |
|                    | 91m | 49.71 min               |                      |                      | Y-x; IT; $\gamma$ (0.556)                                      |
|                    | 91  | 58.5 d                  |                      | 1.4(3)               | $\beta^-$ (1.545); $\gamma$ (1.21)                             |
|                    | 92  | 3.54 h                  |                      |                      | $\beta^-$ (3.64); $\gamma$ (0.448, 0.561, 0.934, 1.405)        |
|                    | 93  | 10.2 h                  |                      |                      | $\beta^-$ (2.88); $\gamma$ (0.267, 0.947, 1.918)               |
| Zirconium          | 86  | 16.5 h                  |                      |                      | K, Y-x; $\gamma$ (0.243, 0.612)                                |
|                    | 87  | 1.73 h                  |                      |                      | $\beta^+$ (2.260); K, Y-x; $\gamma$ (0.381, 1.228)             |
|                    | 88  | 83.4 d                  |                      |                      | K, Y-x; $\gamma$ (0.393)                                       |
|                    | 89  | 3.27 d                  |                      |                      | K, $\beta^+$ (0.897); Y-x; $\gamma$ (0.909)                    |
|                    | 91  |                         | 11.22(4)             | 1.2(3)               |                                                                |
|                    | 93  | $1.5 \times 10^6$ y     |                      |                      | $\beta^-$ (0.091)                                              |
|                    | 95  | 64.02 d                 |                      |                      | $\beta^-$ (0.366, 0.400); $\gamma$ (0.724, 0.757)              |
|                    | 97  | 16.90 h                 |                      |                      | $\beta^-$ (1.91); $\gamma$ (0.743)                             |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element    | A   | Half-life            | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                  |
|------------|-----|----------------------|----------------------|----------------------|------------------------------------------------------------------|
| Niobium    | 89  | 2.03 h               |                      |                      | $\beta^+$ (3.320); $\gamma$ (1.627)                              |
|            | 90  | 14.60 h              |                      |                      | $\beta^+$ (1.50); K, Zr-x; $\gamma$ (0.141, 1.129, 2.186, 2.319) |
|            | 91m | 62 d                 |                      |                      | IT, Nb-x; $\gamma$ (0.1045, 1.205)                               |
|            | 91  | 700 y                |                      |                      | Mo-x                                                             |
|            | 92m | 10.15 d              |                      |                      | K, $\gamma$ (0.913, 0.934, 1.848)                                |
|            | 93m | 16.1 y               |                      |                      | Nb-x                                                             |
|            | 93  |                      | 100                  | 1.1                  |                                                                  |
|            | 94m | 6.26 min             |                      |                      | $\gamma$ (0.871)                                                 |
|            | 94  | $2.4 \times 10^4$ y  |                      |                      | $\beta^-$ (0.473); $\gamma$ (0.703, 0.871)                       |
|            | 95m | 3.61 d               |                      |                      | $\gamma$ (0.204, 0.236)                                          |
|            | 95  | 35.0 d               |                      | < 7                  | $\beta^-$ (0.160); $\gamma$ (0.765)                              |
|            | 96  | 23.4 h               |                      |                      | $\beta^-$ (0.748, 0.500); $\gamma$ (0.778, 1.091)                |
|            | 97m | 58.1 s               |                      |                      | IT; $\gamma$ (0.766)                                             |
|            | 97  | 1.23 h               |                      |                      | $\beta^-$ (1.267); $\gamma$ (0.481, 0.658)                       |
| Molybdenum | 90  | 5.67 h               |                      |                      | K, $\beta^+$ (1.085); Nb-x; $\gamma$ (0.122, 0.257)              |
|            | 93m | 6.85 h               |                      |                      | IT, Mo-x; $\gamma$ (0.264, 0.685, 1.477)                         |
|            | 95  |                      | 15.92(5)             | 13.4(5)              |                                                                  |
|            | 97  |                      | 9.55(3)              | 2.5(3)               |                                                                  |
|            | 98  |                      | 24.13(7)             | 0.14(1)              |                                                                  |
|            | 99  | 2.75 d               |                      |                      | $\beta^-$ (1.357); Tc-x; $\gamma$ (0.181, 0.366, 0.739)          |
|            | 101 | 14.6 min             |                      |                      | $\beta^-$ (2.23, 0.7); $\gamma$ (0.192, 0.591)                   |
| Technetium | 93  | 2.73 h               |                      |                      | $\beta^+$ (0.81); $\gamma$ (1.363, 1.477, 1.520)                 |
|            | 94  | 4.88 h               |                      |                      | $\beta^+$ (4.256); $\gamma$ (0.449, 0.703, 0.850, 0.871)         |
|            | 95m | 61 d                 |                      |                      | $\beta^+$ (0.71); $\gamma$ (0.204, 0.582, 0.835)                 |
|            | 95  | 20.0 h               |                      |                      | K, Mo-x; $\gamma$ (0.766, 1.074)                                 |
|            | 96  | 4.3 d                |                      |                      | K, Mo-x; $\gamma$ (0.778, 0.813, 0.850, 1.122)                   |
|            | 97m | 90 d                 |                      |                      | K, Tc-x; $\gamma$ (0.0965)                                       |
|            | 97  | $2.6 \times 10^6$ y  |                      |                      | K, Mo-x                                                          |
|            | 98  | $4.2 \times 10^6$ y  |                      |                      | $\beta^-$ (0.40); $\gamma$ (0.652, 0.745)                        |
|            | 99m | 6.012 h              |                      |                      | IT, Tc-x; $\gamma$ (0.141, 0.143)                                |
|            | 99  | $2.13 \times 10^5$ y |                      | 20                   | $\beta^-$ (0.292)                                                |
| Ruthenium  | 95  | 1.64 h               |                      |                      | $\beta^+$ (1.20, 0.91); $\gamma$ (0.290, 0.336, 0.627)           |
|            | 97  | 2.88 d               |                      |                      | K, Tc-x; $\gamma$ (0.216, 0.324, 0.461)                          |
|            | 100 |                      | 12.6(1)              | 5.8(6)               |                                                                  |

TABLE 4.16 Table of Nuclides (Continued)

| Element              | A    | Half-life           | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                                        |
|----------------------|------|---------------------|----------------------|----------------------|----------------------------------------------------------------------------------------|
| Ruthenium<br>(cont.) | 101  |                     | 17.0(1)              | 5.(1)                |                                                                                        |
|                      | 102  |                     | 31.6(2)              | 1.2(1)               |                                                                                        |
|                      | 103  | 39.27 d             |                      | <20                  | $\beta^-$ (0.12, 0.223); $\gamma$ (0.295, 0.4444, 0.497, 0.557, 0.610)                 |
|                      | 105  | 4.44 h              |                      |                      | $\beta^-$ (1.187, 0.11, 1.134); $\gamma$ (0.149, 0.263, 0.317, 0.469, 0.676, 0.724)    |
|                      | 106  | 1.020 y             |                      |                      | $\beta^-$ (0.0394)                                                                     |
| Rhodium              | 99m  | 4.7 h               |                      |                      | $\beta^+$ (0.74); $\gamma$ (0.277, 0.341, 0.618, 1.261)                                |
|                      | 99   | 16 d                |                      |                      | $\beta^+$ (0.54, 0.68); $\gamma$ (0.089, 0.353, 0.528)                                 |
|                      | 100  | 20.8 h              |                      |                      | $\beta^+$ (2.62, 2.07); $\gamma$ (0.446, 0.540, 0.588, 0.823, 1.553, 2.376)            |
|                      | 101m | 4.35 d              |                      |                      | K, IT, Ru-x, Rh-x; $\gamma$ (0.127, 0.307, 0.545)                                      |
|                      | 101  | 3.3 y               |                      |                      | K, Ru-x; $\gamma$ (0.127, 0.198, 0.325)                                                |
|                      | 102m | 207 d               |                      |                      | $\beta^-$ (1.15); $\beta^+$ (1.29, 0.82); $\gamma$ (0.469, 0.475, 0.557, 0.628, 1.103) |
|                      | 102  | 2.9 y               |                      |                      | K, Ru-x; $\gamma$ (0.475, 0.631, 0.697, 0.767, 1.047, 1.103)                           |
|                      | 103m | 56.12 min           |                      |                      | IT, Rh-x, $\gamma$ (0.0.040)                                                           |
|                      | 103  |                     | 100                  | 145                  |                                                                                        |
|                      | 104m | 4.36 min            |                      | 800.(100)            | $\gamma$ (0.051, 0.097, 0.556)                                                         |
|                      | 104  | 42.3 s              |                      | 40.(30)              | $\beta^-$ (2.44), $\gamma$ (0.358, 0.556, 1.237)                                       |
|                      | 105m | 40 s                |                      |                      | IT, Rh-x; $\gamma$ (0.130)                                                             |
|                      | 105  | 35.4 h              |                      | $1.1(3) \times 10^4$ | $\beta^-$ (0.567, 0.247); $\gamma$ (0.280, 0.306, 0.319)                               |
|                      | 106m | 2.18 h              |                      |                      | $\beta^-$ (0.92); $\gamma$ (0.222, 0.451, 0.512, 0.616, 0.717, 0.784, 1.046, 1.528)    |
|                      | 106  | 29.80 s             |                      |                      | $\beta^-$ (3.54, 3.0, 2.4); $\gamma$ (0.512, 0.622)                                    |
| Palladium            | 100  | 3.63 d              |                      |                      | K, Rh-x; $\gamma$ (0.0748, 0.0840, 0.0327)                                             |
|                      | 101  | 8.47 h              |                      |                      | K, Rh-x; $\beta^+$ (0.776); $\gamma$ (0.296, 0.590)                                    |
|                      | 103  | 16.99 d             |                      |                      | K, Rh-x; $\gamma$ (0.357, 0.497)                                                       |
|                      | 105  |                     | 22.33(8)             | 22.(2)               |                                                                                        |
|                      | 107  | $6.5 \times 10^6$ y |                      | 1.8(2)               | $\beta^-$ (0.03)                                                                       |
|                      | 108  |                     | 26.46(9)             | 8.7                  |                                                                                        |
|                      | 109  | 13.5 h              |                      |                      | $\beta^-$ (1.028); Ag-x; $\gamma$ (0.088, 0.311, 0.636)                                |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                       | A            | Half-life            | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                             |
|-------------------------------|--------------|----------------------|----------------------|----------------------|-----------------------------------------------------------------------------|
| Palladium<br>( <i>cont.</i> ) | 111 <i>m</i> | 5.5 h                |                      |                      | $\beta^-$ (0.35, 0.77); $\gamma$ (0.070, 0.172, 0.391)                      |
|                               | 111          | 23.4 min             |                      |                      | $\beta^-$ (2.2); $\gamma$ (0.060, 0.245, 0.580, 0.650, 1.389, 1.459)        |
|                               | 112          | 21.4 h               |                      |                      | $\beta^-$ (0.28); $\gamma$ (0.018)                                          |
| Silver                        | 103          | 1.10 h               |                      |                      | $\beta^+$ (1.7, 1.3); $\gamma$ (0.119, 0.148)                               |
|                               | 104          | 69 min               |                      |                      | $\beta^+$ (0.99); $\gamma$ (0.556, 0.926, 0.942)                            |
|                               | 105          | 41.29 d              |                      |                      | K, Pd-x; $\gamma$ (0.064, 0.280, 0.344, 0.443)                              |
|                               | 106 <i>m</i> | 8.4 d                |                      |                      | K, Pd-x; $\gamma$ (0.451, 0.512, 0.717, 1.046)                              |
|                               | 107 <i>m</i> | 44.2 s               |                      |                      | K, Ag-x; $\gamma$ (0.093)                                                   |
|                               | 107          |                      | 51.839(7)            | 35                   |                                                                             |
|                               | 108 <i>m</i> | 130 y                |                      |                      | $\gamma$ (0.434, 0.614, 0.723)                                              |
|                               | 108          | 2.42 min             |                      |                      | $\beta^-$ (1.65); $\beta^+$ (0.90); $\gamma$ (0.434, 0.619, 0.633)          |
|                               | 109          |                      | 48.161(7)            | 91                   |                                                                             |
|                               | 110 <i>m</i> | 249.8 d              |                      | 82.(11)              | $\beta^-$ (0.087, 0.530); IT, $\gamma$ (0.658, 0.764, 0.885, 0.937, 1.384)  |
|                               | 111 <i>m</i> | 1.08 min             |                      |                      | K, Ag-x; $\gamma$ (0.060, 0.245)                                            |
| Cadmium                       | 111          | 7.47 d               |                      | 3.(2)                | $\beta^-$ (1.04); $\gamma$ (0.245, 0.342)                                   |
|                               | 112          | 3.13 h               |                      |                      | $\beta^-$ (3.94, 3.4); $\gamma$ (0.607, 0.617, 1.39)                        |
|                               | 107          | 6.52 h               |                      |                      | $\beta^+$ (0.302); K, Ag-x; $\gamma$ (0.093, 0.829)                         |
|                               | 109          | 462 d                |                      |                      | K, Ag-x; $\gamma$ (0.088)                                                   |
|                               | 111 <i>m</i> | 48.5 min             |                      |                      | K, Cd-x; $\gamma$ (0.151, 0.245)                                            |
|                               | 111          |                      | 12.80(8)             | 24.(3)               |                                                                             |
|                               | 113 <i>m</i> | 14.1 y               |                      |                      | $\beta^-$ (0.59); $\gamma$ (0.264)                                          |
|                               | 113          | $9 \times 10^{15}$ y | 12.22(6)             | 20 060.(40)          |                                                                             |
|                               | 115 <i>m</i> | 44.6 d               |                      |                      | $\beta^-$ (1.62); $\gamma$ (0.934, 1.29, 0.485)                             |
|                               | 115          | 2.228 d              |                      |                      | $\beta^-$ (1.11, 0.593); In-x; $\gamma$ (0.231, 0.260, 0.336, 0.492, 0.528) |
|                               | 117 <i>m</i> | 3.4 h                |                      |                      | $\beta^-$ (0.72); $\gamma$ (0.159, 0.553); In-x                             |
| Indium                        | 117          | 2.49 h               |                      |                      | $\beta^-$ (0.67, 2.2); $\gamma$ (0.221, 0.273, 0.345, 1.303)                |
|                               | 109          | 4.2 h                |                      |                      | K, Cd-x; $\beta^+$ (0.79); $\gamma$ (0.203, 0.623)                          |
|                               | 110 <i>m</i> | 4.9 h                |                      |                      | $\gamma$ (0.658, 0.885, 0.937)                                              |
|                               | 110          | 1.15 h               |                      |                      | $\beta^+$ (2.22); K, Cd-x; $\gamma$ (0.658)                                 |
|                               | 111          | 2.805 d              |                      |                      | K, Cd-x; $\gamma$ (0.171, 0.245)                                            |

TABLE 4.16 Table of Nuclides (Continued)

| Element           | A    | Half-life              | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                                   |
|-------------------|------|------------------------|----------------------|----------------------|-----------------------------------------------------------------------------------|
| Indium<br>(cont.) | 113m | 1.658 h                |                      |                      | IT, In-x; $\gamma$ (0.392)                                                        |
|                   | 114m | 49.51 d                |                      |                      | IT, K, In-x; $\gamma$ (0.190)                                                     |
|                   | 114  | 1.1983 min             |                      |                      | $\beta^-$ (1.99); K, Cd-x, $\beta^+$ (0.40); $\gamma$ (0.558, 0.573, 1.30)        |
|                   | 115m | 4.486 h                |                      |                      | $\beta^-$ (0.83); K, In-x; $\gamma$ (0.336, 0.497)                                |
|                   | *115 | $4.4 \times 10^{14}$ y | 95.71(2)             | 205                  | $\beta^-$ (0.495)                                                                 |
|                   | 116m | 54.1 min               |                      |                      | $\beta^-$ (1.00); $\gamma$ (0.138, 0.417, 1.09, 1.293)                            |
|                   | 117m | 1.94 h                 |                      |                      | $\beta^-$ (1.77); $\gamma$ (0.159, 0.315, 0.553)                                  |
|                   | 117  | 44 min                 |                      |                      | $\beta^-$ (0.74); $\gamma$ (0.159, 0.397, 0.553)                                  |
| Tin               | 110  | 4.1 h                  |                      |                      | K, In-x; $\gamma$ (0.283)                                                         |
|                   | 113  | 115.1 d                |                      | $\approx 9$          | K, In-x, $\gamma$ (0.392, 0.255)                                                  |
|                   | 116  |                        | 14.53(11)            | 1.1(1)               |                                                                                   |
|                   | 117m | 13.60 d                |                      |                      | K, Sn-x; $\gamma$ (0.159)                                                         |
|                   | 119m | 293 d                  |                      |                      | K, Se-x; $\gamma$ (0.239)                                                         |
|                   | 119  |                        | 8.59(4)              | 2.(1)                |                                                                                   |
|                   | 121m | $\approx 55$ y         |                      |                      | $\beta^-$ (0.354); K, In-x; $\gamma$ (0.0372)                                     |
|                   | 121  | 1.128 d                |                      |                      | $\beta^-$ (0.383)                                                                 |
|                   | 123  | 129.2 d                |                      |                      | $\beta^-$ (1.42); $\gamma$ (0.160, 1.030, 1.089)                                  |
|                   | 125  | 9.63 d                 |                      |                      | $\beta^-$ (2.35); $\gamma$ (1.067)                                                |
| Antimony          | 127  | 2.10 h                 |                      |                      | $\beta^-$ (2.42, 3.2); $\gamma$ (0.823, 1.096)                                    |
|                   | 115  | 32.1 min               |                      |                      | $\beta^+$ (1.51); $\gamma$ (0.499)                                                |
|                   | 116m | 1.00 h                 |                      |                      | $\beta^+$ (1.16); $\gamma$ (0.407, 0.543, 0.973, 1.293)                           |
|                   | 117  | 2.80 h                 |                      |                      | $\beta^+$ (0.57); $\gamma$ (0.159)                                                |
|                   | 118m | 5.00 h                 |                      |                      | $\gamma$ (0.254, 1.051, 1.280)                                                    |
|                   | 118  | 3.6 min                |                      |                      | $\beta^+$ (2.65); $\gamma$ (1.230)                                                |
|                   | 119  | 38.1 h                 |                      |                      | $\gamma$ (0.0239)                                                                 |
|                   | 120  | 15.89 min              |                      |                      | $\beta^+$ (1.72); $\gamma$ (0.704, 1.171)                                         |
|                   | 121  |                        | 57.21(5)             | 6                    |                                                                                   |
|                   | 122  | 2.72 d                 |                      |                      | $\beta^-$ (1.414); $\beta^+$ (1.980); $\gamma$ (0.564, 0.693, 1.141, 1.257)       |
|                   | 123  |                        | 42.7(9)              | 3.3                  |                                                                                   |
|                   | 124  | 60.20 d                |                      |                      | $\beta^-$ (0.61, 2.301); $\gamma$ (0.603, 0.646, 1.69, 0.723)                     |
|                   | 126  | 12.4 d                 |                      |                      | $\beta^-$ (1.9); $\gamma$ (0.279, 0.415, 0.666, 0.695, 0.720)                     |
|                   | 127  | 3.84 d                 |                      |                      | $\beta^-$ (0.89, 1.10, 1.50); $\gamma$ (0.252, 0.291, 0.412, 0.437, 0.686, 0.784) |
|                   | 128  | 9.1 h                  |                      |                      | $\beta^-$ (2.3); $\gamma$ (0.215, 0.314, 0.527, 0.743, 0.754)                     |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                      | A            | Half-life           | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                                                           |
|------------------------------|--------------|---------------------|----------------------|----------------------|-----------------------------------------------------------------------------------------------------------|
| Antimony<br>( <i>cont.</i> ) | 129          | 4.40 h              |                      |                      | $\beta^-$ (0.65); $\gamma$ (0.181, 0.359, 0.460, 0.545, 0.813, 0.915, 1.030)                              |
| Tellurium                    | 116          | 2.49 h              |                      |                      | $\gamma$ (0.0937)                                                                                         |
|                              | 117          | 1.03 h              |                      |                      | $\beta^+$ (1.78); $\gamma$ (0.920, 1.716, 2.300)                                                          |
|                              | 119 <i>m</i> | 4.69 d              |                      |                      | $\gamma$ (0.154, 0.271, 1.213)                                                                            |
|                              | 119          | 16.0 h              |                      |                      | $\beta^+$ (0.627); $\gamma$ (0.644, 0.700)                                                                |
|                              | 121 <i>m</i> | $\approx 154$ d     |                      |                      | $\gamma$ (0.212)                                                                                          |
|                              | 121          | 16.8 d              |                      |                      | $\gamma$ (0.508, 0.573)                                                                                   |
|                              | 123 <i>m</i> | 119.7 d             |                      |                      | $\gamma$ (0.159)                                                                                          |
|                              | 125          |                     | 7.139(6)             | 1.6(2)               |                                                                                                           |
|                              | 127 <i>m</i> | 109 d               |                      |                      | $\beta^-$ (0.77); $\gamma$ (0.088)                                                                        |
|                              | 127          | 9.35 h              |                      |                      | $\beta^-$ (0.696); $\gamma$ (0.360)                                                                       |
|                              | 129 <i>m</i> | 33.6 d              |                      |                      | $\beta^-$ (1.60); $\gamma$ (0.460, 0.696)                                                                 |
|                              | 129          | 1.160 h             |                      |                      | $\beta^-$ (1.453, 0.989); I-x, $\gamma$ (0.460, 0.487)                                                    |
|                              | 131 <i>m</i> | 1.35 d              |                      |                      | $\beta^-$ (0.42); IT, Te-x, I-x; $\gamma$ (0.150, 0.774, 0.794, 0.852)                                    |
|                              | 131          | 25.0 min            |                      |                      | $\beta^-$ (2.14, 1.69, 1.35); I-x; $\gamma$ (0.150, 0.453, 0.493)                                         |
|                              | 132          | 25.0 min            |                      |                      | $\beta^-$ (0.215); $\gamma$ (0.050, 0.112, 0.228)                                                         |
| Iodine                       | 121          | 2.12 h              |                      |                      | $\beta^+$ (1.2); $\gamma$ (2.12)                                                                          |
|                              | 122          | 3.6 min             |                      |                      | $\beta^+$ (3.1); $\gamma$ (0.564)                                                                         |
|                              | 123          | 13.2 h              |                      |                      | K, Te-x; $\gamma$ (0.159)                                                                                 |
|                              | 124          | 4.18 d              |                      |                      | $\beta^+$ (1.54, 2.14, 0.75); $\gamma$ (0.603, 0.723, 1.691)                                              |
|                              | 125          | 59.4 d              |                      | $9.(1) \times 10^2$  | K, Te-x; $\gamma$ (0.035)                                                                                 |
|                              | 126          | 13.0 d              |                      |                      | $\beta^+$ (1.13); $\beta^-$ (0.87, 1.25); $\gamma$ (0.389, 0.662)                                         |
|                              | 127          |                     | 100                  | 6.15(10)             |                                                                                                           |
|                              | 128          | 24.99 min           |                      | 22.(4)               | $\beta^-$ (2.13); $\gamma$ (0.443, 0.527)                                                                 |
|                              | 129          | $1.7 \times 10^7$ y |                      |                      | $\beta^-$ (0.15); $\gamma$ (0.040)                                                                        |
|                              | 130          | 12.36 h             |                      | 18.(3)               | $\beta^+$ (1.13); $\beta^-$ (0.87, 1.25); $\gamma$ (0.389, 0.662)                                         |
|                              | 131          | 8.040 d             |                      | $\approx 0.7$        | $\beta^-$ (0.606); $\gamma$ (0.284, 0.364, 0.637)                                                         |
|                              | 132          | 208 h               |                      |                      | $\beta^-$ (0.80, 1.03, 1.2, 1.6, 2.16); $\gamma$ (0.098, 0.506, 0.523, 0.630, 0.651, 0.667, 0.723, 0.955) |
|                              | 133          | 20.8 h              |                      |                      | $\beta^-$ (1.24); $\gamma$ (0.511, 0.530, 0.875)                                                          |
|                              | 135          | 6.57 h              |                      |                      | $\beta^-$ (0.9, 1.3); $\gamma$ (0.418, 0.527, 1.132, 1.260)                                               |
| Xenon                        | 123          | 2.00 h              |                      |                      | $\beta^+$ (1.51); $\gamma$ (0.149, 0.178)                                                                 |
|                              | 125          | 17.1 h              |                      |                      | $\gamma$ (0.188, 0.243)                                                                                   |

TABLE 4.16 Table of Nuclides (Continued)

| Element                | A            | Half-life           | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                    |
|------------------------|--------------|---------------------|----------------------|----------------------|--------------------------------------------------------------------|
| Xenon ( <i>cont.</i> ) | 127 <i>m</i> | 1.15 min            |                      |                      | $\gamma$ (0.127, 0.173)                                            |
|                        | 127          | 36.4 d              |                      |                      | $\gamma$ (0.172, 0.203, 0.375)                                     |
|                        | 129 <i>m</i> | 8.89 d              |                      |                      | $\gamma$ (0.040, 0.197)                                            |
|                        | 129          |                     | 26.4(6)              | 22.(5)               |                                                                    |
|                        | 131 <i>m</i> | 11.9 d              |                      |                      | $\gamma$ (0.164)                                                   |
|                        | 131          |                     | 21.2(4)              | 90.(10)              |                                                                    |
|                        | 133 <i>m</i> | 2.19 d              |                      |                      | $\gamma$ (0.233)                                                   |
|                        | 133          | 5.243 d             |                      | 190.(90)             | $\beta^-$ (0.346); Cs-x;<br>$\gamma$ (0.081)                       |
|                        | 135 <i>m</i> | 15.3 min            |                      |                      | $\gamma$ (0.527)                                                   |
|                        | 135          | 9.1 h               |                      |                      | $\beta^-$ (0.91); $\gamma$ (0.250, 0.608)                          |
| Cesium                 | 126          | 1.64 min            |                      |                      | $\beta^+$ (3.4, 3.7); $\gamma$ (0.0389, 0.491, 0.925)              |
|                        | 127          | 6.2 h               |                      |                      | $\beta^+$ (0.65, 1.06); $\gamma$ (0.125, 0.412)                    |
|                        | 128          | 3.62 min            |                      |                      | $\beta^+$ (2.44, 2.88); $\gamma$ (0.443)                           |
|                        | 129          | 1.336 d             |                      |                      | $\gamma$ (0.372, 0.412)                                            |
|                        | 132          | 6.48 d              |                      |                      | $\gamma$ (0.465, 0.630, 0.668)                                     |
|                        | 133          |                     | 100                  | 28                   |                                                                    |
|                        | 134 <i>m</i> | 2.91 h              |                      |                      | IT, K, Cs-x; $\gamma$ (0.127)                                      |
|                        | 134          | 2.065 y             |                      | 140.(10)             | $\beta^-$ (0.658, 0.089);<br>$\gamma$ (0.563, 0.569, 0.605, 0.796) |
|                        | 135          | $2.3 \times 10^6$ y |                      | 8.9(5)               | $\beta^-$ (0.205)                                                  |
|                        | 136          | 13.16 d             |                      |                      | $\beta^-$ (0.341); $\gamma$ (0.341, 0.819, 1.048)                  |
| Barium                 | 137          | 30.2 y              |                      |                      | $\beta^-$ (0.514); K, Ba-x;<br>$\gamma$ (0.662)                    |
|                        | 126          | 1.65 h              |                      |                      | $\gamma$ (0.218, 0.234, 0.258)                                     |
|                        | 128          | 2.43 d              |                      |                      | $\gamma$ (0.273); K, Cs-x                                          |
|                        | 129 <i>m</i> | 2.17 h              |                      |                      | $\gamma$ (0.177, 0.182, 0.202, 1.459)                              |
|                        | 129          | 2.2 h               |                      |                      | $\beta^+$ (1.42); $\gamma$ (0.129, 0.214, 0.221)                   |
|                        | 131          | 11.7 d              |                      |                      | $\gamma$ (0.124, 0.216, 0.496)                                     |
|                        | 133 <i>m</i> | 1.621 d             |                      |                      | $\gamma$ (0.276)                                                   |
|                        | 133          | 10.53 y             |                      | 4.(1)                | $\gamma$ (0.081, 0.356)                                            |
|                        | 135 <i>m</i> | 1.196 d             |                      |                      | IT, Ba-x; $\gamma$ (0.268)                                         |
|                        | 135          |                     | 6.59(2)              | 5.8                  |                                                                    |
|                        | 137          |                     | 11.23(4)             | 5.(1)                |                                                                    |
|                        | 137 <i>m</i> | 2.552 min           |                      |                      | IT, K, Ba-x; $\gamma$ (0.662)                                      |
|                        | 138          |                     | 71.70(7)             | 0.41(2)              |                                                                    |
|                        | 139          | 1.396 h             |                      | 5.1                  | $\beta^-$ (2.27, 2.14); K, La-x;<br>$\gamma$ (0.166, 1.254, 1.421) |
|                        | 140          | 12.75 d             |                      |                      | $\beta^-$ (0.48, 1.02); $\gamma$ (0.163, 0.305, 0.537)             |
|                        | 142          | 10.7 min            |                      |                      | $\beta^-$ (1.0, 1.1); $\gamma$ (0.231, 0.255, 0.309, 1.204)        |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element      | A    | Half-life               | Natural abundance, % | Cross section, barns | Radiation (MeV)                                            |
|--------------|------|-------------------------|----------------------|----------------------|------------------------------------------------------------|
| Lanthanum    | 131  | 59 min                  |                      |                      | $\beta^+$ (1.42, 1.94); $\gamma$ (0.526, 0.109, 0.366)     |
|              | 132  | 4.8 h                   |                      |                      | $\beta^+$ (2.6, 3.2, 3.7); $\gamma$ (0.465, 0.567)         |
|              | 133  | 3.91 h                  |                      |                      | $\beta^+$ (1.2); $\gamma$ (0.279, 0.290, 0.302)            |
|              | 134  | 6.5 min                 |                      |                      | $\beta^+$ (2.67); $\gamma$ (0.605)                         |
|              | 135  | 19.5 h                  |                      |                      | $\gamma$ (0.481)                                           |
|              | 136  | 8.87 min                |                      |                      | $\beta^+$ (1.8); $\gamma$ (0.816)                          |
|              | *138 | $1.06 \times 10^{11}$ y |                      | 57.(6)               |                                                            |
|              | 139  |                         | 99.9098(2)           | 9.2(2)               |                                                            |
|              | 140  | 1.68 d                  |                      | 2.7(3)               | $\beta^-$ (1.670, 1.35)                                    |
|              | 141  | 3.90 h                  |                      |                      | $\beta^-$ (2.43)                                           |
| Cerium       | 142  | 1.54 h                  |                      |                      | $\beta^-$ (2.11, 2.98, 4.52)                               |
|              | 132  | 3.5 h                   |                      |                      | $\gamma$ (0.154, 0.182)                                    |
|              | 133  | 5.4 h                   |                      |                      | $\beta^+$ (1.3); $\gamma$ (0.058, 0.131, 0.472, 0.510)     |
|              | 135  | 17.7 h                  |                      |                      | $\beta^+$ (0.8); $\gamma$ (0.266, 0.300, 0.607)            |
|              | 137m | 1.43 d                  |                      |                      | IT K, Ce-x; $\gamma$ (0.169, 0.254)                        |
|              | 137  | 9.0 h                   |                      |                      | $\gamma$ (0.447)                                           |
|              | 139  | 137.6 d                 |                      |                      | $\gamma$ (0.166)                                           |
|              | 140  |                         | 88.43(10)            | 0.58(4)              |                                                            |
|              | 141  | 32.50 d                 |                      |                      | $\beta^-$ (0.436, 0.581); K, Pr-x; $\gamma$ (0.145)        |
|              | 142  |                         | 11.13(10)            | 0.97(3)              |                                                            |
| Praseodymium | 143  | 1.38 d                  |                      | 6.1(7)               | $\beta^-$ (1.404, 1.110); K, Pr-x; $\gamma$ (0.293)        |
|              | 144  | 284.6 d                 |                      | 1.0(1)               | $\beta^-$ (0.318, 0.185); K, Pr-x; $\gamma$ (0.080, 0.134) |
|              | 136  | 13.1 min                |                      |                      | $\beta^+$ (2.98); $\gamma$ (0.540, 0.552)                  |
|              | 137  | 1.28 h                  |                      |                      | $\beta^+$ (1.68); $\gamma$ (0.434, 0.514, 0.837)           |
|              | 138m | 2.1 h                   |                      |                      | $\beta^+$ (1.65); $\gamma$ (0.304, 0.789, 1.038)           |
|              | 139  | 4.41 h                  |                      |                      | $\beta^+$ (1.09); $\gamma$ (0.255, 1.347, 1.631)           |
|              | 141  |                         | 100                  | 11.5                 |                                                            |
|              | 142  | 19.12 h                 |                      | 20.(3)               | $\beta^-$ (2.164); $\gamma$ (1.576)                        |
|              | 143  | 13.57 d                 |                      | 90.(10)              | $\beta^-$ (0.933); $\gamma$ (0.742)                        |
|              | 145  | 5.98 h                  |                      |                      | $\beta^-$ (1.80); $\gamma$ (0.073, 0.676, 0.748)           |
| Neodymium    | 139m | 5.5 h                   |                      |                      | $\beta^+$ (1.17); $\gamma$ (0.114, 0.738)                  |
|              | 141  | 2.49 h                  |                      |                      | $\beta^+$ (0.802)                                          |
|              | 142  |                         | 27.13(2)             | 19.(1)               |                                                            |
|              | 143  |                         | 12.18(6)             | 220.(10)             |                                                            |
|              | *144 | $2.1 \times 10^{15}$ y  | 23.8(1)              | 3.6(3)               |                                                            |
|              | 145  |                         | 8.3(6)               | 47.(6)               |                                                            |



TABLE 4.16 Table of Nuclides (Continued)

| Element              | A    | Half-life               | Natural abundance, % | Cross section, barns  | Radiation (MeV)                                                              |
|----------------------|------|-------------------------|----------------------|-----------------------|------------------------------------------------------------------------------|
| Neodymium<br>(cont.) | 146  |                         | 17.19(9)             | 1.5(2)                |                                                                              |
|                      | 147  | 10.98 d                 |                      | 440.(150)             | $\beta^-$ (0.805); $\gamma$ (0.091, 0.531)                                   |
|                      | 149  | 1.73 h                  |                      |                       | $\beta^-$ (1.03, 1.13); $\gamma$ (0.211, 0.114)                              |
| Promethium           | 143  | 265 d                   |                      |                       | K, Nd-x; $\gamma$ (0.742)                                                    |
|                      | 144  | 360 d                   |                      |                       | K, Nd-x; $\gamma$ (0.618, 0.696)                                             |
|                      | 146  | 5.53 y                  |                      | $8.4(2) \times 10^3$  | K, $\beta^-$ (0.795); Nd-x; $\gamma$ (0.453, 0.75)                           |
|                      | 147  | 2.6234 y                |                      | 180                   | $\beta^-$ (0.224); $\gamma$ (0.122, 0.197)                                   |
|                      | 148m | 41.29 d                 |                      | $106.(8) \times 10^2$ | $\beta^-$ (0.69, 0.50, 0.40); IT, Pm-x, Sm-x; $\gamma$ (0.550, 0.630, 0.726) |
|                      | 148  | 5.37 d                  |                      | $\approx 1000$        | $\beta^-$ (1.02, 2.47); $\gamma$ (0.550, 0.915, 1.465)                       |
|                      | 149  | 2.212 d                 |                      | $14.(2) \times 10^2$  | $\beta^-$ (1.072, 0.78); $\gamma$ (0.286, 0.591, 0.859)                      |
|                      | 150  | 2.68 h                  |                      |                       | $\beta^-$ (1.6, 2.3, 1.8); $\gamma$ (0.334, 1.166, 0.132)                    |
|                      | 151  | 1.183 d                 |                      | $\approx 150$         | $\beta^-$ (0.84); $\gamma$ (0.168, 0.275, 0.340)                             |
| Samarium             | 142  | 1.208 h                 |                      |                       | $\beta^+$ (1.0); K, Pr-x                                                     |
|                      | 144  |                         | 3.1(1)               | 1.6(1)                |                                                                              |
|                      | 145  | 340 d                   |                      | 280.(20)              | $\gamma$ (0.061, 0.492); K, Pm-x                                             |
|                      | 146  | $1.03 \times 10^8$ y    |                      |                       | $\alpha$ (2.50)                                                              |
|                      | *147 | $1.06 \times 10^{11}$ y | 15.0(2)              | 56.(4)                | $\alpha$ (2.23)                                                              |
|                      | 148  | $7 \times 10^{15}$ y    | 11.3(1)              | 2.4(6)                | $\alpha$ (1.96)                                                              |
|                      | 149  | $10^{16}$ y             | 13.8(1)              | $401.(6) \times 10^2$ |                                                                              |
|                      | 150  |                         | 7.4(1)               | 102.(5)               |                                                                              |
|                      | 151  | 90 y                    |                      |                       | $\beta^-$ (0.076)                                                            |
|                      | 152  |                         | 26.7(2)              | 206.(15)              |                                                                              |
|                      | 153  | 1.929 d                 |                      | 420.(180)             | $\beta^-$ (0.64, 0.69); $\gamma$ (0.103)                                     |
|                      | 154  |                         | 22.7(2)              | 7.5(3)                |                                                                              |
| Europium             | 155  | 22.2 min                |                      |                       | $\beta^-$ (1.52); $\gamma$ (0.104)                                           |
|                      | 156  | 9.4 h                   |                      |                       | $\beta^-$ (0.43, 0.71); $\gamma$ (0.166, 0.204)                              |
|                      | 148  | 54.5 d                  |                      |                       | $\beta^+$ (0.92); $\gamma$ (0.550, 0.630)                                    |
|                      | 149  | 93.1 d                  |                      |                       | K, Sm-x; $\gamma$ (0.277, 0.328)                                             |
|                      | 150m | 12.8 h                  |                      |                       | $\beta^-$ (1.013); $\gamma$ (0.334, 0.407)                                   |
|                      | 150  | 36 y                    |                      |                       | $\gamma$ (0.334, 0.439, 0.584)                                               |
|                      | 151  |                         | 47.8(5)              | 9000                  |                                                                              |
|                      | 152m | 9.30 h                  |                      |                       | $\beta^-$ (1.85); $\gamma$ (0.122, 0.841, 0.963)                             |
|                      | 152  | 13.48 y                 |                      | $11.(2) \times 10^3$  | K, $\beta^-$ (1.47, 0.690); K, Gd-x, K, Sm-x; $\gamma$ (0.122, 0.344, 1.408) |
|                      | 153  |                         | 52.2(5)              | 320.(20)              |                                                                              |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                      | A    | Half-life           | Natural abundance, % | Cross section, barns   | Radiation (MeV)                                                          |
|------------------------------|------|---------------------|----------------------|------------------------|--------------------------------------------------------------------------|
| Europium<br>( <i>cont.</i> ) | 154  | 8.59 y              |                      | $1.5(3) \times 10^3$   | $\beta^-$ (0.27, 0.58, 0.843, 1.87); $\gamma$ (0.123, 0.723, 1.274)      |
|                              | 155  | 4.76 y              |                      | $3.9(2) \times 10^3$   | $\beta^-$ (0.15); $\gamma$ (0.087, 0.105)                                |
|                              | 156  | 15.2 d              |                      |                        | $\beta^-$ (0.30, 0.49, 1.2, 2.45); $\gamma$ (0.089, 0.646, 0.723, 0.812) |
|                              | 157  | 15.13 h             |                      |                        | $\beta^-$ (1.30); $\gamma$ (0.064, 0.371, 0.411)                         |
|                              | 158  | 45.9 min            |                      |                        | $\beta^-$ (2.5); $\gamma$ (0.898, 0.944, 0.977)                          |
| Gadolinium                   | 146  | 48.3 d              |                      |                        | $\beta^+$ (0.35); $\gamma$ (0.115, 0.155)                                |
|                              | 147  | 1.588 d             |                      |                        | $\beta^+$ (0.93); $\gamma$ (0.229, 0.370, 0.396, 0.929)                  |
|                              | 151  | 124 d               |                      |                        | $\alpha$ (2.73); $\gamma$ (0.154, 0.243)                                 |
|                              | 153  | 241.6 d             |                      |                        | $\gamma$ (0.94, 0.103)                                                   |
|                              | 155  |                     | 14.80(5)             | $61.(1) \times 10^3$   |                                                                          |
|                              | 157  |                     | 15.65(3)             | $2.54(3) \times 10^5$  |                                                                          |
|                              | 158  |                     | 24.84(12)            | 2.3(5)                 |                                                                          |
|                              | 159  | 18.56 h             |                      |                        | $\beta^-$ (0.971); Tb-x; $\gamma$ (0.363)                                |
| Terbium                      | 160  |                     | 21.86(4)             | 1.5(7)                 |                                                                          |
|                              | 158  | 180 y               |                      |                        | $\gamma$ (0.944, 0.962)                                                  |
|                              | 159  |                     | 100                  | 23.2(5)                |                                                                          |
| Dysprosium                   | 160  | 72.3 d              |                      | $5.7(11) \times 10^2$  | $\beta^-$ (0.57, 0.86); $\gamma$ (0.299, 0.879, 0.966)                   |
|                              | 159  | 144 d               |                      | $8.(2) \times 10^3$    | K, Tb-x; $\gamma$ (0.326)                                                |
|                              | 161  |                     | 18.9(2)              | 600.(150)              |                                                                          |
|                              | 162  |                     | 25.5(2)              | 170.(20)               |                                                                          |
|                              | 163  |                     | 24.9(2)              | 120.(10)               |                                                                          |
|                              | 164  |                     | 28.2(2)              | 2000                   |                                                                          |
|                              | 165  | 2.33 h              |                      | $3.5(3) \times 10^3$   | $\beta^-$ (1.29); Ho-x; $\gamma$ (0.095)                                 |
|                              | 165m | 1.26 min            |                      |                        | $\gamma$ (0.108, 0.515)                                                  |
| Holmium                      | 156  | 56 min              |                      |                        | $\gamma$ (0.138, 0.267)                                                  |
|                              | 159  | 33.0 min            |                      |                        | $\gamma$ (0.121, 0.132, 0.253, 0.310)                                    |
|                              | 167  | 3.1 h               |                      |                        | $\beta^-$ (0.31, 0.62, 0.96); $\gamma$ (0.238, 0.321, 0.347)             |
|                              | 165  |                     | 100                  | 61                     |                                                                          |
|                              | 166m | $1.2 \times 10^3$ y |                      | $9.14(65) \times 10^3$ | Er-x; $\gamma$ (0.810, 0.712, 0.184)                                     |
|                              | 166  | 1.117 d             |                      |                        | $\beta^-$ (1.855, 1.776); $\gamma$ (1.379)                               |
| Erbium                       | 166  |                     | 33.6(2)              | 20                     |                                                                          |
|                              | 167  |                     | 22.95(15)            | $7.(2) \times 10^2$    |                                                                          |
|                              | 168  |                     | 26.8(2)              | 2.0(6)                 |                                                                          |
|                              | 169  | 9.40 d              |                      |                        | $\beta^-$ (0.35)                                                         |
|                              | 170  |                     | 14.9(2)              | 6.2(2)                 |                                                                          |

TABLE 4.16 Table of Nuclides (Continued)

| Element                 | A                | Half-life              | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                    |
|-------------------------|------------------|------------------------|----------------------|----------------------|--------------------------------------------------------------------|
| Erbium ( <i>cont.</i> ) | 171              | 7.52 h                 |                      | 370.(40)             | $\beta^-$ (1.49); Tm-x; $\gamma$ (0.112, 0.296, 0.308)             |
|                         | 172              | 2.05 d                 |                      |                      | $\beta^-$ (0.28, 0.36); $\gamma$ (0.407, 0.610)                    |
| Thullium                | 166              | 7.70 h                 |                      |                      | $\gamma$ (0.184, 0.779, 1.273, 2.052)                              |
|                         | 169              |                        | 100                  | 106                  |                                                                    |
|                         | 170              | 128.6 d                |                      | 100.(20)             | $\beta^-$ (0.968, 0.884)                                           |
|                         | 171              | 1.92 y                 |                      | $\approx 160$        | $\beta^-$ (0.096); $\gamma$ (0.067)                                |
|                         | 172              | 2.65 d                 |                      |                      | $\beta^-$ (1.79, 1.86); $\gamma$ (1.387, 1.466, 1.530, 1.609)      |
|                         | 173              | 8.2 h                  |                      |                      | $\beta^-$ (0.80, 0.86); $\gamma$ (0.399, 0.461)                    |
| Ytterbium               | 165              | 9.9 min                |                      |                      | $\beta^+$ (1.58); $\gamma$ (1.090)                                 |
|                         | 166              | 2.363 d                |                      |                      | $\gamma$ (0.184, 0.779, 1.273, 2.052)                              |
|                         | 169              | 32.03 d                |                      | $3.6(3) \times 10^3$ | $\gamma$ (0.110, 0.177, 0.198)                                     |
|                         | 171              |                        | 14.3(2)              | 50.(10)              |                                                                    |
|                         | 173              |                        | 16.12(21)            | 16.(2)               |                                                                    |
|                         | 174              |                        | 31.8(4)              | 120                  |                                                                    |
|                         | 175              | 4.19 d                 |                      |                      | $\beta^-$ (0.466); Lu-x; $\gamma$ (0.396)                          |
|                         | 176              |                        | 12.7(2)              | 3.1(2)               |                                                                    |
|                         | 177              | 1.9 h                  |                      |                      | $\beta^-$ (1.40); K, Lu-x; $\gamma$ (0.150)                        |
| Lutetium                | 178              | 1.23 h                 |                      |                      | $\beta^-$ (0.25); $\gamma$ (0.141, 0.325, 0.352, 0.381, 0.613)     |
|                         | 164              | 3.14 min               |                      |                      | $\beta^+$ (1.6, 3.8); $\gamma$ (0.124, 0.262, 0.740, 0.864, 0.880) |
|                         | 165              | 16.7 min               |                      |                      | $\beta^+$ (2.06); $\gamma$ (0.121, 0.132, 0.174, 0.204)            |
|                         | 175              |                        | 97.41(2)             | 24                   |                                                                    |
|                         | 176 $m$          | 3.66 h                 |                      |                      | $\beta^-$ (1.229, 1.317); Hf-x; $\gamma$ (0.0884)                  |
|                         | 176              | $3.8 \times 10^{16}$ y |                      | 2100                 | $\gamma$ (0.202, 0.307)                                            |
| Hafnium                 | 177              | 6.75 d                 |                      | $10.(3) \times 10^2$ | $\beta^-$ (0.497), Hf-x; $\gamma$ (0.113, 0.208)                   |
|                         | 178              |                        | 27.297(4)            | 85                   |                                                                    |
|                         | 179              |                        | 13.629(6)            | 46                   |                                                                    |
|                         | $\dagger 179m_1$ | 18.7 s                 |                      |                      | $\gamma$ (0.161, 0.214)                                            |
|                         | $\dagger 179m_2$ | 25.1 d                 |                      |                      | $\gamma$ (0.123, 0.146, 0.363, 0.454)                              |
|                         | 180              |                        | 35.100(7)            | 13.(1)               |                                                                    |
|                         | 180 $m$          | 5.519 h                |                      |                      | IT, Hf-x; $\gamma$ (0.215, 0.332, 0.443)                           |
|                         | 181              | 42.4 d                 |                      | 30.(25)              | $\beta^-$ (0.408); Ta-x; $\gamma$ (0.133, 0.346, 0.482)            |

$\dagger$  Two different metastable states possessing the same mass number but different half-lives.

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                     | A       | Half-life            | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                              |
|-----------------------------|---------|----------------------|----------------------|----------------------|------------------------------------------------------------------------------|
| Hafnium<br>( <i>cont.</i> ) | 183     | 1.07 h               |                      |                      | $\beta^-$ (1.18, 1.54); $\gamma$ (0.459, 0.784)                              |
|                             | 184     | 4.1 h                |                      |                      | $\beta^-$ (0.74, 0.85, 1.10); $\gamma$ (0.139, 0.345)                        |
| Tantalum                    | 181     |                      | 99.988(2)            | 20                   |                                                                              |
|                             | 182 $m$ | 16.5 min             |                      |                      | $\gamma$ (0.147, 0.172, 0.184)                                               |
|                             | 182     | 114.43 d             |                      | $8.2(6) \times 10^3$ | $\beta^-$ (0.25, 0.44, 0.52); $\gamma$ (0.068, 1.121)                        |
|                             | 183     | 5.1 d                |                      |                      | $\beta^-$ (0.62); $\gamma$ (0.108, 0.246, 0.304)                             |
|                             | 184     | 8.7 h                |                      |                      | $\beta^-$ (1.17); $\gamma$ (0.253, 0.414)                                    |
| Tungsten                    | 182     |                      | 26.50(3)             | 20.(1)               |                                                                              |
|                             | 183     |                      | 14.31(1)             | 10.5(3)              |                                                                              |
|                             | 184     |                      | 30.64(1)             | 2                    |                                                                              |
|                             | 185     | 74.8 d               |                      | $\approx 3.3$        | $\beta^-$ (0.433); $\gamma$ (0.125)                                          |
|                             | 186     |                      | 28.43(4)             | 37.(2)               |                                                                              |
|                             | 187     | 23.9 h               |                      | 70.(10)              | $\beta^-$ (1.315, 0.624; K, Re-x; $\gamma$ (0.072, 0.480, 0.686)             |
|                             | 188     | 69.4 d               |                      |                      | $\beta^-$ (0.349); $\gamma$ (0.227, 0.291)                                   |
| Rhenium                     | 182 $m$ | 12.7 h               |                      |                      | $\beta^+$ (0.55, 1.74); $\gamma$ (1.121, 1.221)                              |
|                             | 184     | 38 d                 |                      |                      | $\gamma$ (0.790, 0.903)                                                      |
|                             | 185     |                      | 37.40(2)             | 110                  |                                                                              |
|                             | 186     | 3.718 d              |                      |                      | $\beta^-$ (1.07, 0.933); K, W-x, Os-x; $\gamma$ (0.123, 0.137, 0.632, 0.768) |
|                             | *187    | $4.2 \times 10^{10}$ | 62.60(2)             | 74                   |                                                                              |
|                             | 188     | 16.94 h              |                      |                      | $\beta^-$ (2.12, 1.96); Os-x; $\gamma$ (0.155)                               |
|                             | 189     | 24 h                 |                      |                      | $\beta^-$ (1.01); $\gamma$ (0.147, 0.22, 0.245)                              |
| Osmium                      | 186     | $2 \times 10^{15}$ y | 1.58(2)              | $\approx 80$         |                                                                              |
|                             | 188     |                      | 13.3(1)              | $\approx 5$          |                                                                              |
|                             | 190 $m$ | 9.9 min              |                      |                      | IT, Os-x; $\gamma$ (0.187, 0.361, 0.503, 0.616)                              |
|                             | 190     |                      | 26.4(2)              | 13                   |                                                                              |
|                             | 191     | 15.4 d               |                      | $3.8(6) \times 10^2$ | $\beta^-$ (0.143); Os-x; $\gamma$ (0.129)                                    |
|                             | 192     |                      | 41.0(3)              | 3.(1)                |                                                                              |
|                             | 193     | 30.5 h               |                      |                      | $\beta^-$ (1.04); Ir-x; $\gamma$ (0.139, 0.460)                              |
|                             | 196     | 34.9 min             |                      |                      | $\beta^-$ (0.84); $\gamma$ (0.126, 0.408)                                    |
| Iridium                     | 184     | 3.0 h                |                      |                      | $\beta^+$ (2.3, 2.9); $\gamma$ (0.120, 0.264, 0.390)                         |
|                             | 185     | 14 h                 |                      |                      | $\gamma$ (0.254, 1.829)                                                      |
|                             | 186     | 15.7 h               |                      |                      | $\gamma$ (0.137, 0.296, 0.435)                                               |
|                             | 188     | 1.72 d               |                      |                      | $\gamma$ (0.155, 0.478, 0.633, 2.215)                                        |

TABLE 4.16 Table of Nuclides (Continued)

| Element            | A    | Half-life | Natural abundance, % | Cross section, barns   | Radiation (MeV)                                                |
|--------------------|------|-----------|----------------------|------------------------|----------------------------------------------------------------|
| Iridium<br>(cont.) | 189  | 13.2 d    |                      |                        | K, Os-x; $\gamma$ (0.245)                                      |
|                    | 190  | 11.8 d    |                      |                        | $\gamma$ (0.187, 0.407, 0.519, 0.558, 0.605)                   |
|                    | 191  |           | 37.27(9)             | 920                    |                                                                |
|                    | 192  | 73.83 d   |                      |                        | $\beta^-$ (0.672); K, Pt-x; $\gamma$ (0.316, 0.468)            |
|                    | 193  |           | 62.73(9)             | 116                    |                                                                |
|                    | 194  | 19.3 h    |                      | $1.5(3) \times 10^3$   | $\beta^-$ (2.25); $\gamma$ (0.294, 0.328, 0.645)               |
|                    | 195m | 3.9 h     |                      |                        | $\beta^-$ (0.41, 0.97); $\gamma$ (0.320, 0.365, 0.433, 0.685)  |
|                    |      |           |                      |                        |                                                                |
| Platinum           | 187  | 2.35 h    |                      |                        | $\gamma$ (0.105, 0.110, 0.201, 0.285, 0.709)                   |
|                    | 188  | 10.2 d    |                      |                        | $\gamma$ (0.188, 0.195)                                        |
|                    | 189  | 10.89 h   |                      |                        | K, Ir-x; $\gamma$ (0.094, 0.608, 0.721)                        |
|                    | 194  |           | 32.9(6)              | 1.2                    |                                                                |
|                    | 195m | 4.02 d    |                      |                        | IT, Pt-x; $\gamma$ (0.099)                                     |
|                    | 195  |           | 33.8(6)              | 28.(1)                 |                                                                |
|                    | 196  |           | 25.3(6)              | 55                     |                                                                |
|                    | 197m | 1.573 h   |                      |                        | IT, Pt-x; $\gamma$ (0.053, 0.346)                              |
|                    | 197  | 18.3 h    |                      |                        | $\beta^-$ (0.719); K, Au-x; $\gamma$ (0.191, 0.269)            |
|                    | 199m | 14.1 s    |                      |                        | $\gamma$ (0.392)                                               |
| Gold               | 199  | 30.8 min  |                      | $\approx 16$           | $\beta^-$ (0.90, 1.14); $\gamma$ (0.186, 0.317, 0.494, 0.549)  |
|                    | 200  | 12.5 h    |                      |                        | $\gamma$ (0.136, 0.227, 0.244)                                 |
|                    | 197  |           | 100                  | 98.7(1)                |                                                                |
|                    | 197m | 7.8 s     |                      |                        | IT, K, Au-x; $\gamma$ (0.130, 0.279)                           |
|                    | 198  | 2.694 d   |                      | $26.5(15) \times 10^3$ | $\beta^-$ (0.961); K, Hg-x; $\gamma$ (0.412)                   |
|                    | 199  | 3.139 d   |                      |                        | $\beta^-$ (0.292, 0.250); K, Hg-x; $\gamma$ (0.158, 0.208)     |
|                    | 200m | 18.7 h    |                      |                        | $\beta^-$ (0.56); $\gamma$ (0.111, 0.368, 0.498, 0.597, 0.760) |
|                    | 200  | 48.4 min  |                      |                        | $\beta^-$ (2.2); $\gamma$ (0.368, 1.225)                       |
| Mercury            | 196  |           | 0.15(1)              | 3150                   |                                                                |
|                    | 197m | 23.8 h    |                      |                        | IT, K, Hg-x; $\gamma$ (0.134)                                  |
|                    | 197  | 2.6725 d  |                      |                        | K, Au-x; $\gamma$ (0.077)                                      |
|                    | 199m | 42.6 min  |                      |                        | $\gamma$ (0.158)                                               |
|                    | 199  |           | 16.87(10)            | $2.1(2) \times 10^3$   |                                                                |
|                    | 200  |           | 23.10(16)            | $<60$                  |                                                                |
|                    | 202  |           | 29.86(20)            | 4.9(5)                 |                                                                |
| Thallium           | 203  | 46.61 d   |                      |                        | $\beta^-$ (0.213); $\gamma$ (0.279)                            |
|                    | 201  | 3.040 d   |                      |                        | K, Hg-x; $\gamma$ (0.135, 0.167)                               |
|                    | 202  | 12.23 d   |                      |                        | K, Hg-x; $\gamma$ (0.440)                                      |
|                    | 203  |           | 29.52(1)             | 11.(1)                 |                                                                |
|                    | 204  | 3.78 y    |                      | 22.(2)                 | $\beta^-$ (0.763); K, Hg-x                                     |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                      | A    | Half-life | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                                         |
|------------------------------|------|-----------|----------------------|----------------------|-----------------------------------------------------------------------------------------|
| Thallium<br>( <i>cont.</i> ) | 205  |           | 70.48(1)             | 0.11(2)              |                                                                                         |
|                              | *206 | 4.20 min  |                      |                      | $\beta^-$ (1.53); K, Pb-x;<br>$\gamma$ (0.803)                                          |
|                              | *207 | 4.77 min  |                      |                      | $\beta^-$ (1.43); $\gamma$ (0.897)                                                      |
|                              | 208  | 3.053 min |                      |                      | $\beta^-$ (1.796, 1.28, 1.52);<br>$\gamma$ (0.277, 0.511, 0.583, 0.614)                 |
|                              | 209  | 2.16 min  |                      |                      | $\beta^-$ (1.8); $\gamma$ (1.567, 0.465)                                                |
|                              | 210  | 1.30 min  |                      |                      | $\beta^-$ (1.9, 1.3); $\gamma$ (0.298, 0.798)                                           |
| Lead                         | 201  | 9.33 h    |                      |                      | $\gamma$ (0.331, 0.361)                                                                 |
|                              | 203  | 2.1615 d  |                      |                      | $\gamma$ (0.279)                                                                        |
|                              | 204m | 1.120 h   |                      |                      | IT, Pb-x; $\gamma$ (0.375, 0.899, 0.912)                                                |
|                              | 207  |           | 22.1(1)              | 0.70(1)              |                                                                                         |
|                              | 209  | 3.253 h   |                      |                      | $\beta^-$ (0.645)                                                                       |
|                              | *210 | 22.6 y    |                      |                      | $\alpha$ (3.72)                                                                         |
|                              | *211 | 36.1 min  |                      |                      | $\beta^-$ (1.36); $\gamma$ (0.405, 0.427, 0.832)                                        |
|                              | *212 | 10.64 h   |                      |                      | $\beta^-$ (0.569, 0.28); Bi-x;<br>$\gamma$ (0.239)                                      |
|                              | *214 | 26.9 min  |                      |                      | $\beta^-$ (0.67, 0.73); $\gamma$ (0.24, 0.30, 0.352)                                    |
|                              |      |           |                      |                      | $\gamma$ (0.703, 1.764)                                                                 |
| Bismuth                      | 205  | 15.31 d   |                      |                      | $\gamma$ (0.516, 0.803, 0.881)                                                          |
|                              | 206  | 6.243 d   |                      |                      |                                                                                         |
|                              | 209  |           | 100                  | 0.034                |                                                                                         |
|                              | *210 | 5.013 d   |                      |                      | $\beta^-$ (1.16); $\gamma$ (0.266, 0.352)                                               |
|                              | 212  | 1.0092 h  |                      |                      | $\beta^-$ (2.25); $\gamma$ (0.288, 0.727, 0.786, 1.621); Tl-x;<br>$\alpha$ (6.05, 6.09) |
|                              | *214 | 19.7 min  |                      |                      | $\beta^-$ (3.26); $\gamma$ (0.609, 1.120, 1.764)                                        |
| Polonium                     | 204  | 3.53 h    |                      |                      | $\gamma$ (0.270, 0.884, 1.016)                                                          |
|                              | 205  | 1.7 h     |                      |                      | $\gamma$ (0.837, 0.850, 0.872, 1.001)                                                   |
|                              | 206  | 8.8 d     |                      |                      | $\alpha$ (5.233); $\gamma$ (0.286, 0.312, 0.807)                                        |
|                              | 208  | 2.898 y   |                      |                      | $\alpha$ (5.116)                                                                        |
|                              | 209  | 102 y     |                      |                      | $\alpha$ (4.88); IT, K, Bi-x;<br>$\gamma$ (0.260, 0.896)                                |
|                              | 210  | 138.38 d  |                      |                      | $\alpha$ (5.304); $\gamma$ (0.803)                                                      |
|                              | 212  | 298 ns    |                      |                      | $\alpha$ (8.784)                                                                        |
|                              | 214  | 0.1637 ms |                      |                      | $\alpha$ (7.686)                                                                        |
|                              | 216  | 145 ms    |                      |                      | $\alpha$ (6.778)                                                                        |
|                              | 218  | 3.04 min  |                      |                      | $\alpha$ (5.18)                                                                         |
| Astatine                     | 207  | 1.81 h    |                      |                      | $\alpha$ (5.76); $\gamma$ (0.168, 0.588, 0.814)                                         |
|                              | 208  | 1.63 h    |                      |                      | $\alpha$ (5.641); K, Po-x,<br>$\gamma$ (0.177, 0.660, 0.685, 0.845, 1.028)              |

TABLE 4.16 Table of Nuclides (Continued)

| Element             | A    | Half-life                | Natural abundance, % | Cross section, barns | Radiation (MeV)                                                                            |
|---------------------|------|--------------------------|----------------------|----------------------|--------------------------------------------------------------------------------------------|
| Astatine<br>(cont.) | 209  | 5.41 h                   |                      |                      | $\alpha$ (5.65), K, Po-x;<br>$\gamma$ (0.545, 0.782, 0.790)                                |
|                     | 210  | 8.1 h                    |                      |                      | K, Po-x; $\gamma$ (0.245, 0.528, 1.181, 1.437, 1.483)                                      |
|                     | 211  | 7.214 h                  |                      |                      | $\alpha$ (5.87); K, Po-x;<br>$\gamma$ (0.669, 0.742)                                       |
| Radon               | 210  | 2.4 h                    |                      |                      | $\alpha$ (6.039); $\gamma$ (0.196, 0.458, 0.571, 0.649)                                    |
|                     | 211  | 14.68 h                  |                      |                      | $\alpha$ (5.784, 5.851); $\gamma$ (0.169, 0.250, 0.370, 0.674, 0.678, 1.363)               |
|                     | 212  | 24 min                   |                      |                      | $\alpha$ (6.260)                                                                           |
|                     | 220  | 55.6 s                   |                      |                      | $\alpha$ (6.288)                                                                           |
| Francium            | 222  | 2.8235 d                 |                      | 0.74(5)              | $\alpha$ (5.49); $\gamma$ (0.510)                                                          |
|                     | 212  | 20 min                   |                      |                      | $\alpha$ (6.41, 6.26); $\gamma$ (1.186, 1.275)                                             |
|                     | 220  | 27.4 s                   |                      |                      | $\alpha$ (6.686, 0.641, 6.582);<br>$\gamma$ (0.106, 0.154, 0.162)                          |
|                     | 221  | 4.8 min                  |                      |                      | $\alpha$ (6.341); $\gamma$ (0.218, 0.409)                                                  |
|                     | 222  | 14.3 min                 |                      |                      | $\beta^-$ (0.178)                                                                          |
|                     | 223  | 22.0 min                 |                      |                      | $\beta^-$ (0.117)                                                                          |
|                     |      |                          |                      |                      |                                                                                            |
| Radium              | *224 | 3.66 d                   |                      | 12.0(5)              | $\alpha$ (5.685, 5.45); K, Rn-x;<br>$\gamma$ (0.241, 0.409, 0.650)                         |
|                     | *226 | 1599 y                   |                      | $\approx 13$         | $\alpha$ (4.78, 4.60); K, Rn-x;<br>$\gamma$ (0.186, 0.262)                                 |
|                     | *228 | 5.76 y                   |                      | 36.(5)               | $\gamma$ (0.0135)                                                                          |
| Actinium            | *227 | 21.77 y                  |                      | $8.8(7) \times 10^2$ | $\beta^-$ (0.045); $\alpha$ (4.95, 4.94);<br>K, Th-x; $\gamma$ (0.084, 0.160, 0.270)       |
|                     | *228 | 6.15 h                   |                      |                      | $\beta^-$ (2.18, 1.85, 1.11); K,<br>Th-x; $\gamma$ (0.339, 0.911, 0.969)                   |
| Thorium             | 226  | 30.6 min                 |                      |                      | $\alpha$ (6.337, 6.228); $\gamma$ (0.206, 0.242)                                           |
|                     | 228  | 1.913 y                  |                      | $1.2(2) \times 10^2$ | $\alpha$ (5.42, 5.34, 5.18); K,<br>Ra-x                                                    |
|                     | *230 | $7.54 \times 10^4$ y     |                      | 23.4(5)              | $\alpha$ (4.68, 4.62); K, Ra-x;<br>$\gamma$ (0.068)                                        |
|                     | 231  | 1.063 d                  |                      |                      | $\beta^-$ (0.305, 0.218, 0.138)                                                            |
|                     | *232 | $1.405 \times 10^{10}$ y |                      | 7.37(4)              | $\alpha$ (4.01, 3.95); $\gamma$ (0.059)                                                    |
|                     | 233  | 22.3 min                 |                      | $1.5(1) \times 10^3$ | $\beta^-$ (1.245); $\gamma$ (0.459)                                                        |
| Protactinium        | *234 | 24.10 d                  |                      | 1.8(5)               | $\beta^-$ (0.198, 0.102); K,<br>Pa-x                                                       |
|                     | 230  | 17.4 d                   |                      | $1.5(3) \times 10^3$ | $\beta^-$ (0.51); $\gamma$ (0.444, 0.455, 0.899, 0.952)                                    |
|                     | *231 | $3.25 \times 10^4$ y     |                      | $2.0(1) \times 10^2$ | $\alpha$ (5.06, 5.03, 5.01, 4.95, 4.73); K, Ac-x;<br>$\gamma$ (0.260, 0.284, 0.300, 0.330) |

**TABLE 4.16** Table of Nuclides (*Continued*)

| Element                          | A       | Half-life             | Natural abundance, % | Cross section, barns  | Radiation (MeV)                                                                                                 |
|----------------------------------|---------|-----------------------|----------------------|-----------------------|-----------------------------------------------------------------------------------------------------------------|
| Protactinium<br>( <i>cont.</i> ) | 232     | 1.31 d                |                      | $4.6(10) \times 10^2$ | $\beta^-$ (1.34); $\gamma$ (0.109, 0.150, 0.894, 0.969)                                                         |
|                                  | 233     | 27.0 d                |                      |                       | $\beta^-$ (0.256, 0.15, 0.568); K,L U-x; $\gamma$ (0.300, 0.312, 0.341)                                         |
|                                  | 234 $m$ | 1.17 min              |                      |                       | $\beta^-$ (2.29); IT, K, U-x                                                                                    |
| Uranium                          | 235     | 24.4 min              |                      |                       | $\beta^-$ (1.4)                                                                                                 |
|                                  | 230     | 20.8 d                |                      |                       | $\alpha$ (5.89, 5.82)                                                                                           |
|                                  | 232     | 68.9 y                |                      | 73.(2)                | $\alpha$ (5.320, 5.263)                                                                                         |
|                                  | 233     | $1.592 \times 10^5$ y |                      | 47.(2)                | $\alpha$ (4.825, 4.783); L, Th-x; $\gamma$ (0.029, 0.042, 0.055, 0.097, 0.119, 0.146, 0.164, 0.22, 0.291, 0.32) |
|                                  | *234    | $2.454 \times 10^5$ y | 0.0055(5)            | 96.(2)                | $\alpha$ (4.776, 4.723); L, Th-x; $\gamma$ (0.121)                                                              |
|                                  | *235    | $7.037 \times 10^8$ y | 0.720(1)             | 95.(5)                | $\alpha$ (4.40, 4.37, 4.22); K,L Th-x; $\gamma$ (0.14, 0.16, 0.186, 0.20)                                       |
|                                  | 237     | 6.75 d                |                      | $\approx 100$         |                                                                                                                 |
| Neptunium                        | *238    | $4.46 \times 10^9$ y  | 99.2745(15)          | 2.7(1)                | $\alpha$ (4.196, 4.147)                                                                                         |
|                                  | 239     | 23.47 min             |                      | 22.(2)                | $\beta^-$ (1.21, 1.29)                                                                                          |
|                                  | 236     | $1.55 \times 10^5$ y  |                      |                       | $\beta^-$ (0.49), $\gamma$ (0.104, 0.160)                                                                       |
|                                  | 237     | $2.14 \times 10^6$ y  |                      | 180                   | $\alpha$ (4.79, 4.77); K,L Pa-x                                                                                 |
|                                  | 238     | 2.117 d               |                      | 51                    | $\beta^-$ (1.2); $\gamma$ (0.984, 1.029)                                                                        |
| Plutonium                        | 239     | 2.355 d               |                      | $5.1(2) \times 10^2$  | $\beta^-$ (0.438, 0.341); $\gamma$ (0.228, 0.278)                                                               |
|                                  | 237     | 45.7 d                |                      |                       | K,L Np-x                                                                                                        |
|                                  | 238     | 87.74 y               |                      |                       | $\alpha$ (5.50, 5.46); K, U-x; $\gamma$ (0.0435)                                                                |
|                                  | 239     | $2.411 \times 10^4$ y |                      | $2.7(1) \times 10^2$  | $\alpha$ (5.16, 5.14, 5.11); K, U-x; $\gamma$ (0.375, 0.414, 0.129)                                             |
|                                  | 240     | $6.537 \times 10^3$ y |                      | $2.9(1) \times 10^2$  | $\alpha$ (5.168, 5.124); L, U-x                                                                                 |
|                                  | 242     | $3.763 \times 10^5$ y |                      | 19.(1)                | $\alpha$ (4.90, 4.86); $\gamma$ (0.045, 0.103)                                                                  |
|                                  | 244     | $8.2 \times 10^7$ y   |                      | 1.7(1)                | $\alpha$ (4.59, 4.55); L, U-x                                                                                   |
| Americium                        | 246     | 10.85 d               |                      |                       | $\beta^-$ (0.150, 0.35); $\gamma$ (0.224)                                                                       |
|                                  | 241     | 432.2 y               |                      | 600                   | $\alpha$ (5.49, 5.44); $\gamma$ (0.12, 0.14)                                                                    |
|                                  | 243     | 7370 y                |                      | 80                    | $\alpha$ (5.277, 5.234); $\gamma$ (0.075)                                                                       |
| Curium                           | 242     | 162.8 d               |                      | $\approx 20$          | $\alpha$ (6.113, 6.069); L, Pu-x                                                                                |
|                                  | 243     | 28.5 y                |                      | $1.3(1) \times 10^2$  | $\alpha$ (5.786, 5.742)                                                                                         |
|                                  | 244     | 18.11 y               |                      | 15.(1)                | $\alpha$ (5.805, 5.753); $\gamma$ (0.099, 1.526)                                                                |
| Berkelium                        | 247     | $1.4 \times 10^3$ y   |                      |                       | $\alpha$ (5.532, 5.678, 5.712)                                                                                  |
|                                  | 249     | 320 d                 |                      | $7.(1) \times 10^2$   | $\alpha$ (5.42); $\beta^-$ (0.125)                                                                              |
|                                  | 250     | 3.217 h               |                      |                       | $\beta^-$ (0.74); $\gamma$ (0.989, 1.032)                                                                       |



**TABLE 4.16** Table of Nuclides (*Continued*)

| Element     | A   | Half-life | Natural abundance, % | Cross section, barns | Radiation (MeV)                                          |
|-------------|-----|-----------|----------------------|----------------------|----------------------------------------------------------|
| Californium | 251 | 900 y     |                      | $2.9(2) \times 10^2$ | $\alpha(5.677, 5.851, 6.014)$                            |
|             | 252 | 2.645 y   |                      | 20.(2)               | $\alpha(6.118, 6.076)$ ; L, Cm-x; $\gamma(0.043, 0.100)$ |
| Einsteinium | 253 | 20.47 d   |                      | 186                  | $\alpha(6.64)$ ; $\gamma(0.389)$                         |
|             | 254 | 275.7 d   |                      | 28.(3)               | $\alpha(6.43)$                                           |
|             | 255 | 40 d      |                      | $\approx 55$         | $\beta^-(0.29)$ ; $\alpha(6.26)$                         |
| Fermium     | 255 | 20.1 h    |                      | 26.(3)               | $\alpha(7.023)$                                          |
|             | 257 | 100.5 d   |                      |                      | $\alpha(6.519)$ ; L, Cf-x; $\gamma(0.179, 0.241)$        |
| Mendelevium | 258 | 51.5 d    |                      |                      | $\alpha(6.718, 6.763)$ ; $\gamma(0.368)$                 |
|             | 260 | 32 d      |                      |                      |                                                          |
| Nobelium    | 255 | 3.1 min   |                      |                      | $\alpha(8.12, 7.93)$ ; $\gamma(0.187)$                   |
|             | 259 | 58 min    |                      |                      | $\alpha(7.52, 7.55)$                                     |
| Lawrencium  | 260 | 3 min     |                      |                      |                                                          |
|             | 261 | 40 min    |                      |                      |                                                          |
|             | 262 | 3.6 h     |                      |                      |                                                          |

**Source:** R. B. Firestone and V. S. Shirley, eds., *Table of Isotopes*, 8th ed., Wiley, New York, 1997, and V. S. Shirley, ed., *Table of Radioactive Isotopes*, 8th ed., Wiley-Interscience, New York, 1986.

4.9 WORK FUNCTION

**TABLE 4.17** Work Functions of the Elements

The work function  $\phi$  is the energy necessary to just remove an electron from the metal surface in thermoelectric or photoelectric emission. Values are dependent upon the experimental technique (vacua of  $10^{-9}$  or  $10^{-10}$  torr, clean surfaces, and surface conditions including the crystal face identification).

| Element | $\phi$ , eV | Element | $\phi$ , eV |
|---------|-------------|---------|-------------|
| Ag      | 4.64        | Eu      | 2.5         |
| Al      | 4.19        | Fe      | 4.65        |
| As      | (3.75)      | Ga      | 4.25        |
| Au      | 5.32        | Ge      | 5.0         |
| B       | (4.75)      | Gd      | 3.1         |
| Ba      | 2.35        | Hf      | 3.65        |
| Be      | 5.08        | Hg      | 4.50        |
| Bi      | 4.36        | In      | 4.08        |
| C       | (5.0)       | Ir      | 5.6         |
| Ca      | 2.71        | K       | 2.30        |
| Cd      | 4.12        | La      | 3.40        |
| Ce      | 2.80        | Li      | 3.10        |
| Co      | 4.70        | Mg      | 3.66        |
| Cr      | 4.40        | Mn      | 3.90        |
| Cs      | 1.90        | Mo      | 4.30        |
| Cu      | 4.70        | Na      | 2.70        |

**TABLE 4.17** Work Functions of the Elements (*Continued*)

| Element | $\phi$ , eV | Element | $\phi$ , eV |
|---------|-------------|---------|-------------|
| Nb      | 4.20        | Si      | 4.85        |
| Nd      | 3.1         | Sm      | 2.95        |
| Ni      | 5.15        | Sn      | 4.35        |
| Os      | 4.83        | Sr      | 2.76        |
| Pb      | 4.18        | Ta      | 4.22        |
| Pd      | 5.00        | Tb      | 3.0         |
| Po      | 4.6         | Te      | 4.70        |
| Pr      | 2.7         | Th      | 3.71        |
| Pt      | 5.40        | Ti      | 4.10        |
| Rb      | 2.20        | Tl      | 4.02        |
| Re      | 4.95        | U       | 3.70        |
| Rh      | 4.98        | V       | 4.44        |
| Ru      | 4.80        | W       | 4.55        |
| Sb      | 4.56        | Y       | 3.1         |
| Sc      | 3.5         | Zn      | 4.30        |
| Se      | 5.9         | Zr      | 4.00        |

**Source:** S. Trasatti, *J. Chem. Soc. Faraday Trans. I* **68**:229 (1972); N. D. Lang and W. Kohn, *Phys. Rev. B* **3**:1215 (1971).

#### 4.10 RELATIVE ABUNDANCES OF NATURALLY OCCURRING ISOTOPES

**TABLE 4.18** Relative Abundances of Naturally Occurring Isotopes

| Element   | Mass number | Percent   | Element  | Mass number | Percent    |
|-----------|-------------|-----------|----------|-------------|------------|
| Aluminum  | 27          | 100       | Cadmium  | 112         | 24.13(14)  |
| Antimony  | 121         | 57.21(5)  |          | 113         | 12.22(8)   |
|           | 123         | 42.79(5)  |          | 114         | 28.7(3)    |
| Argon     | 36          | 0.337(3)  |          | 116         | 7.49(9)    |
|           | 38          | 0.063(1)  | Calcium  | 40          | 96.941(18) |
|           | 40          | 99.600(3) |          | 42          | 0.647(9)   |
| Arsenic   | 75          | 100       |          | 43          | 0.135(6)   |
| Barium    | 130         | 0.106(2)  |          | 44          | 2.088(12)  |
|           | 132         | 0.101(2)  |          | 46          | 0.004(3)   |
|           | 134         | 2.42(3)   |          | 48          | 0.187(4)   |
|           | 135         | 6.59(2)   | Carbon   | 12          | 98.89(1)   |
|           | 136         | 7.85(4)   |          | 13          | 1.11(1)    |
|           | 137         | 11.23(4)  | Cerium   | 136         | 0.19(1)    |
|           | 138         | 71.70(7)  |          | 138         | 0.25(1)    |
| Beryllium | 9           | 100       |          | 140         | 88.43(10)  |
| Bismuth   | 209         | 100       |          | 142         | 11.13(10)  |
| Boron     | 10          | 19.9(2)   | Cesium   | 133         | 100        |
|           | 11          | 80.1(2)   | Chlorine | 35          | 75.77(7)   |
| Bromine   | 79          | 50.69(7)  |          | 37          | 24.23(7)   |
|           | 81          | 49.31(7)  | Chromium | 50          | 4.345(13)  |
| Cadmium   | 106         | 1.25(4)   |          | 52          | 83.79(2)   |
|           | 108         | 0.89(2)   |          | 53          | 9.50(2)    |
|           | 110         | 12.49(12) |          | 54          | 2.365(7)   |
|           | 111         | 12.80(8)  | Cobalt   | 59          | 100        |

**TABLE 4.18** Relative Abundances of Naturally Occurring Isotopes (*Continued*)

| Element    | Mass<br>number | Percent    | Element    | Mass<br>number | Percent    |
|------------|----------------|------------|------------|----------------|------------|
| Copper     | 63             | 69.17(3)   | Krypton    | 78             | 0.35(2)    |
|            | 65             | 30.83(3)   |            | 80             | 2.25(2)    |
| Dysprosium | 156            | 0.06(1)    | Lanthanum  | 82             | 11.6(1)    |
|            | 158            | 0.10(1)    |            | 83             | 11.5(1)    |
|            | 160            | 2.34(6)    |            | 84             | 57.0(3)    |
|            | 161            | 18.9(2)    |            | 86             | 17.3(2)    |
|            | 162            | 25.5(2)    |            | 138            | 0.0902(2)  |
|            | 163            | 24.9(2)    | Lead       | 139            | 99.9098(2) |
| Erbium     | 164            | 28.2(2)    |            | 204            | 1.4(1)     |
|            | 162            | 0.14(1)    |            | 206            | 24.1(1)    |
|            | 164            | 1.61(2)    |            | 207            | 22.1(1)    |
|            | 166            | 33.6(2)    |            | 208            | 52.4(1)    |
|            | 167            | 22.95(15)  | Lithium    | 6              | 7.5(2)     |
|            | 168            | 26.8(2)    |            | 7              | 92.5(2)    |
| Europium   | 170            | 14.9(2)    | Lutetium   | 175            | 97.41(2)   |
|            | 151            | 47.8(5)    |            | 176            | 2.59(2)    |
|            | 153            | 52.2(5)    | Magnesium  | 24             | 78.99(3)   |
| Fluorine   | 19             | 100        |            | 25             | 10.00(1)   |
| Gadolinium | 152            | 0.20(1)    |            | 26             | 11.01(2)   |
|            | 154            | 2.18(3)    | Manganese  | 55             | 100        |
|            | 155            | 14.80(5)   |            | 196            | 0.15(1)    |
|            | 156            | 20.47(4)   | Mercury    | 198            | 9.97(8)    |
|            | 157            | 15.65(3)   |            | 199            | 16.87(10)  |
|            | 158            | 24.84(12)  |            | 200            | 23.10(16)  |
| Gallium    | 160            | 21.86(4)   |            | 201            | 13.18(8)   |
|            | 69             | 60.108(9)  |            | 202            | 29.86(20)  |
|            | 71             | 39.892(9)  |            | 204            | 6.87(4)    |
|            | 70             | 21.23(4)   | Molybdenum | 92             | 14.84(4)   |
| Germanium  | 72             | 27.66(3)   |            | 94             | 9.25(3)    |
|            | 73             | 7.73(1)    |            | 95             | 15.92(5)   |
|            | 74             | 35.94(2)   |            | 96             | 16.68(5)   |
|            | 76             | 7.44(2)    |            | 97             | 9.55(3)    |
| Gold       | 197            | 100        |            | 98             | 24.13(7)   |
| Hafnium    | 174            | 0.162(3)   |            | 100            | 9.63(3)    |
|            | 176            | 5.206(5)   | Neodymium  | 142            | 27.13(12)  |
|            | 177            | 18.606(13) |            | 143            | 12.18(6)   |
|            | 178            | 27.297(4)  |            | 144            | 23.80(12)  |
|            | 179            | 13.629(6)  |            | 145            | 8.30(6)    |
|            | 180            | 35.100(7)  |            | 146            | 17.19(9)   |
| Helium     | 4              | 100        |            | 148            | 5.76(3)    |
| Holmium    | 165            | 100        |            | 150            | 5.64(3)    |
| Hydrogen   | 1              | 99.985(1)  | Neon       | 20             | 90.48(3)   |
|            | 2              | 0.015(1)   |            | 21             | 0.27(1)    |
| Indium     | 113            | 4.29(2)    |            | 22             | 9.25(3)    |
|            | 115            | 95.71(2)   | Nickel     | 58             | 68.077(9)  |
| Iodine     | 127            | 100        |            | 60             | 26.223(8)  |
| Iridium    | 191            | 37.27(9)   |            | 61             | 1.140(1)   |
|            | 193            | 62.73(9)   |            | 62             | 3.634(2)   |
| Iron       | 54             | 5.85(4)    |            | 64             | 0.926(1)   |
|            | 56             | 91.75(4)   | Niobium    | 93             | 100        |
|            | 57             | 2.12(1)    | Nitrogen   | 14             | 99.634(9)  |
|            | 58             | 0.26(1)    |            | 15             | 0.366(9)   |

**TABLE 4.18** Relative Abundances of Naturally Occurring Isotopes (*Continued*)

| Element       | Mass number | Percent   | Element   | Mass number | Percent    |
|---------------|-------------|-----------|-----------|-------------|------------|
| Osmium        | 184         | 0.020(3)  | Silicon   | 78          | 23.78(9)   |
|               | 186         | 1.58(2)   |           | 80          | 49.61(10)  |
|               | 187         | 1.6(4)    |           | 82          | 8.73(6)    |
|               | 188         | 13.3(1)   |           | 28          | 92.23(2)   |
|               | 189         | 16.1(1)   |           | 29          | 4.67(2)    |
|               | 190         | 26.4(2)   |           | 30          | 3.10(1)    |
|               | 192         | 41.0(3)   | Silver    | 107         | 51.839(7)  |
| Oxygen        | 16          | 99.76(1)  |           | 109         | 48.161(7)  |
|               | 17          | 0.04      | Sodium    | 23          | 100        |
|               | 18          | 0.20(1)   |           | 84          | 0.56(1)    |
| Palladium     | 102         | 1.02(1)   | Strontium | 86          | 9.86(1)    |
|               | 104         | 11.14(8)  |           | 87          | 7.00(1)    |
|               | 105         | 22.33(8)  |           | 88          | 82.58(1)   |
|               | 106         | 27.33(3)  | Sulfur    | 32          | 95.02(9)   |
|               | 108         | 26.46(9)  |           | 33          | 0.75(4)    |
|               | 110         | 11.72(9)  |           | 34          | 4.21(8)    |
| Phosphorus    | 31          | 100       |           | 36          | 0.02(1)    |
| Platinum      | 190         | 0.01(1)   | Tantalum  | 180         | 0.012(2)   |
|               | 192         | 0.79(6)   |           | 181         | 99.988(2)  |
|               | 194         | 32.9(6)   | Tellurium | 120         | 0.096(2)   |
|               | 195         | 33.8(6)   |           | 122         | 2.603(4)   |
|               | 196         | 25.3(6)   |           | 123         | 0.908(2)   |
|               | 198         | 7.2(2)    |           | 124         | 4.816(6)   |
| Potassium     | 39          | 93.258(4) |           | 125         | 7.139(6)   |
|               | 40          | 0.0117(1) |           | 126         | 18.952(11) |
|               | 41          | 6.730(3)  |           | 128         | 31.687(11) |
| Praseodymium  | 141         | 100       |           | 130         | 33.799(10) |
| Protoactinium | 230         | 100       | Terbium   | 159         | 100        |
| Rhenium       | 185         | 37.40(2)  |           | 203         | 29.52(1)   |
|               | 187         | 62.60(2)  | Thallium  | 205         | 70.48(1)   |
| Rhodium       | 103         | 100       |           | 228         | 100        |
| Rubidium      | 85          | 72.17(2)  | Thulium   | 169         | 100        |
|               | 87          | 27.83(2)  |           | 112         | 0.97(1)    |
| Ruthenium     | 96          | 5.52(6)   |           | 114         | 0.65(1)    |
|               | 98          | 1.88(6)   |           | 115         | 0.34(1)    |
|               | 99          | 12.7(1)   |           | 116         | 14.53(11)  |
|               | 100         | 12.6(1)   |           | 117         | 7.68(7)    |
|               | 101         | 17.0(1)   |           | 118         | 24.23(11)  |
|               | 102         | 31.6(2)   |           | 119         | 8.59(4)    |
|               | 104         | 18.7(2)   |           | 120         | 32.59(10)  |
|               | 144         | 3.1(1)    | Titanium  | 122         | 4.63(3)    |
| Samarium      | 147         | 15.0(2)   |           | 124         | 5.79(5)    |
|               | 148         | 11.3(1)   |           | 46          | 8.25(3)    |
|               | 149         | 13.8(1)   |           | 47          | 7.44(2)    |
|               | 150         | 7.4(1)    |           | 48          | 73.72(3)   |
|               | 152         | 26.7(2)   |           | 49          | 5.41(2)    |
|               | 154         | 22.7(2)   |           | 50          | 5.4(1)     |
| Scandium      | 45          | 100       | Tungsten  | 180         | 0.12(1)    |
| Selenium      | 74          | 0.89(2)   |           | 182         | 26.50(3)   |
|               | 76          | 9.36(11)  |           | 183         | 14.31(1)   |
|               | 77          | 6.63(6)   |           | 184         | 30.64(1)   |

**TABLE 4.18** Relative Abundances of Naturally Occurring Isotopes (*Continued*)

| Element                   | Mass<br>number | Percent   | Element   | Mass<br>number | Percent  |
|---------------------------|----------------|-----------|-----------|----------------|----------|
| Tungsten ( <i>cont.</i> ) | 186            | 28.43(4)  |           | 171            | 14.3(2)  |
| Uranium                   | 234            | 0.0055(5) |           | 172            | 21.9(3)  |
|                           | 235            | 0.720(1)  |           | 173            | 16.12(2) |
|                           | 238            | 99.275(2) |           | 174            | 31.8(4)  |
| Vanadium                  | 50             | 0.250(2)  |           | 176            | 12.7(2)  |
|                           | 51             | 99.750(2) | Yttrium   | 89             | 100      |
| Xenon                     | 124            | 0.10(1)   | Zinc      | 64             | 48.6(3)  |
|                           | 126            | 0.09(1)   |           | 66             | 27.9(2)  |
|                           | 128            | 1.91(3)   |           | 67             | 4.1(1)   |
|                           | 129            | 26.4(6)   |           | 68             | 18.8(4)  |
|                           | 130            | 4.1(1)    |           | 70             | 0.6(1)   |
|                           | 131            | 21.2(4)   | Zirconium | 90             | 51.45(3) |
|                           | 132            | 26.9(5)   |           | 91             | 11.22(4) |
|                           | 134            | 10.4(2)   |           | 92             | 17.15(2) |
|                           | 136            | 8.9(1)    |           | 94             | 17.38(4) |
| Ytterbium                 | 168            | 0.13(1)   |           | 96             | 2.80(2)  |
|                           | 170            | 3.05(6)   |           |                |          |

**Source:** A. H. Wapstra and G. Audi, “*The 1983 Atomic Mass Evaluation*,” Nucl. Phys., **A432:1-54** (1985) and references cited for Table 4.16.

---

# SECTION 5

---

## PHYSICAL PROPERTIES

---

|                                                                                                                   |              |
|-------------------------------------------------------------------------------------------------------------------|--------------|
| <b>5.1 SOLUBILITIES</b>                                                                                           | <b>5.3</b>   |
| Table 5.1 Solubility of Gases in Water                                                                            | 5.3          |
| Table 5.2 Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures   | 5.9          |
| <b>5.2 VAPOR PRESSURES</b>                                                                                        | <b>5.24</b>  |
| Table 5.3 Vapor Pressure of Mercury                                                                               | 5.24         |
| Table 5.4 Vapor Pressure of Ice in Millimeters of Mercury                                                         | 5.26         |
| Table 5.5 Vapor Pressure of Liquid Ammonia, NH <sub>3</sub>                                                       | 5.27         |
| Table 5.6 Vapor Pressure of Water                                                                                 | 5.28         |
| Table 5.7 Vapor Pressure of Deuterium Oxide                                                                       | 5.29         |
| <b>5.2.1 Vapor-Pressure Equations</b>                                                                             | <b>5.30</b>  |
| Table 5.8 Vapor Pressures of Various Inorganic Compounds                                                          | 5.31         |
| Table 5.9 Vapor Pressures of Various Organic Compounds                                                            | 5.39         |
| <b>5.3 BOILING POINTS</b>                                                                                         | <b>5.57</b>  |
| Table 5.10 Boiling Points of Water                                                                                | 5.57         |
| Table 5.11 Binary Azeotropic (Constant-Boiling) Mixtures                                                          | 5.58         |
| Table 5.12 Ternary Azeotropic Mixtures                                                                            | 5.77         |
| <b>5.4 FREEZING MIXTURES</b>                                                                                      | <b>5.83</b>  |
| Table 5.13 Compositions of Aqueous Antifreeze Solutions                                                           | 5.83         |
| <b>5.4.1 Propylene Glycol–Glycerol</b>                                                                            | <b>5.86</b>  |
| <b>5.5 DENSITY AND SPECIFIC GRAVITY</b>                                                                           | <b>5.87</b>  |
| Table 5.14 Density of Mercury and Water                                                                           | 5.87         |
| Table 5.15 Specific Gravity of Air at Various Temperatures                                                        | 5.88         |
| <b>5.5.1 Density of Moist Air</b>                                                                                 | <b>5.88</b>  |
| <b>5.5.2 Specific Gravity Corrections for the Buoyant Effect of Air</b>                                           | <b>5.89</b>  |
| <b>5.6 VISCOSITY, SURFACE TENSION, DIELECTRIC CONSTANT, DIPOLE MOMENT, AND REFRACTIVE INDEX</b>                   | <b>5.90</b>  |
| Table 5.16 Viscosity and Surface Tension of Various Organic Substances                                            | 5.90         |
| Table 5.17 Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances                     | 5.105        |
| Table 5.18 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances    | 5.130        |
| Table 5.19 Refractive Index, Viscosity, Dielectric Constant, and Surface Tension of Water at Various Temperatures | 5.134        |
| <b>5.6.1 Refractive Index</b>                                                                                     | <b>5.135</b> |
| Table 5.20 Atomic and Group Refractions                                                                           | 5.136        |
| <b>5.6.2 Surface Tension</b>                                                                                      | <b>5.136</b> |
| <b>5.6.3 Dipole Moments</b>                                                                                       | <b>5.136</b> |
| <b>5.6.4 Dielectric Constants</b>                                                                                 | <b>5.137</b> |
| <b>5.6.5 Viscosity</b>                                                                                            | <b>5.137</b> |
| Table 5.21 Aqueous Glycerol Solutions                                                                             | 5.138        |
| Table 5.22 Aqueous Sucrose Solutions                                                                              | 5.138        |
| <b>5.7 COMBUSTIBLE MIXTURES</b>                                                                                   | <b>5.139</b> |
| Table 5.23 Properties of Combustible Mixtures in Air                                                              | 5.139        |
| <b>5.8 THERMAL CONDUCTIVITY</b>                                                                                   | <b>5.148</b> |
| Table 5.24 Thermal Conductivities of Gases as a Function of Temperature                                           | 5.148        |
| Table 5.25 Liquid Thermal Conductivity of Various Substances                                                      | 5.151        |
| Table 5.26 Thermal Conductivity of Various Solids                                                                 | 5.154        |

|                                                          |              |
|----------------------------------------------------------|--------------|
| <b>5.9 MISCELLANY</b>                                    | <b>5.155</b> |
| Table 5.27 Compressibility of Water                      | 5.155        |
| Table 5.28 Mass of Water Vapor in Saturated Air          | 5.156        |
| Table 5.29 Van der Waals' Constants for Gases            | 5.157        |
| Table 5.30 Triple Points of Various Materials            | 5.168        |
| <b>5.9.1 Some Physical Chemistry Equations for Gases</b> | <b>5.169</b> |

5.1 SOLUBILITIES

TABLE 5.1 Solubility of Gases in Water

The column (or line entry) headed “ $\alpha$ ” gives the volume of gas (in milliliters) measured at standard conditions (0°C and 760 mm or 101.325 kN · m<sup>-2</sup>) dissolved in 1 mL of water at the temperature stated (in degrees Celsius) and when the pressure of the gas without that of the water vapor is 760 mm. The line entry “A” indicates the same quantity except that the gas itself is at the uniform pressure of 760 mm when in equilibrium with water.

The column headed “1” gives the volume of the gas (in milliliters) dissolved in 1 mL of water when the pressure of the gas plus that of the water vapor is 760 mm.

The column headed “q” gives the weight of gas (in grams) dissolved in 100 g of water when the pressure of the gas plus that of the water vapor is 760 mm.

| Temp.<br>°C | Acetylene |       | Air*                  |                    | Ammonia  |      | Bromine  |      |
|-------------|-----------|-------|-----------------------|--------------------|----------|------|----------|------|
|             | $\alpha$  | q     | $\alpha(\times 10^3)$ | % oxygen<br>in air | $\alpha$ | q    | $\alpha$ | q    |
| 0           | 1.73      | 0.200 | 29.18                 | 34.91              | 1130     | 89.5 | 60.5     | 42.9 |
| 1           | 1.68      | 0.194 | 28.42                 | 34.87              | —        | —    | —        | —    |
| 2           | 1.63      | 0.188 | 27.69                 | 34.82              | —        | —    | 54.1     | 38.3 |
| 3           | 1.58      | 0.182 | 26.99                 | 34.78              | —        | —    | —        | —    |
| 4           | 1.53      | 0.176 | 26.32                 | 34.74              | 1047     | 79.6 | 48.3     | 34.2 |
| 5           | 1.49      | 0.171 | 25.68                 | 34.69              | —        | —    | —        | —    |
| 6           | 1.45      | 0.167 | 25.06                 | 34.65              | —        | —    | 43.3     | 30.6 |
| 7           | 1.41      | 0.162 | 24.47                 | 34.60              | —        | —    | —        | —    |
| 8           | 1.37      | 0.157 | 23.90                 | 34.56              | 947      | 72.0 | 38.9     | 27.5 |
| 9           | 1.34      | 0.154 | 23.36                 | 34.52              | —        | —    | —        | —    |
| 10          | 1.31      | 0.150 | 22.84                 | 34.47              | 870      | 68.4 | 35.1     | 24.8 |
| 11          | 1.27      | 0.146 | 22.34                 | 34.43              | —        | —    | —        | —    |
| 12          | 1.24      | 0.142 | 21.87                 | 34.38              | 857      | 65.1 | 31.5     | 22.2 |
| 13          | 1.21      | 0.138 | 21.41                 | 34.34              | 837      | 63.6 | —        | —    |
| 14          | 1.18      | 0.135 | 20.97                 | 34.30              | —        | —    | 28.4     | 20.0 |
| 15          | 1.15      | 0.131 | 20.55                 | 34.25              | 770      | —    | —        | —    |
| 16          | 1.13      | 0.129 | 20.14                 | 34.21              | 775      | 58.7 | 25.7     | 18.0 |
| 17          | 1.10      | 0.125 | 19.75                 | 34.17              | —        | —    | —        | —    |
| 18          | 1.08      | 0.123 | 19.38                 | 34.12              | —        | —    | 23.4     | 16.4 |
| 19          | 1.05      | 0.119 | 19.02                 | 34.08              | —        | —    | —        | —    |
| 20          | 1.03      | 0.117 | 18.68                 | 34.03              | 680      | 52.9 | 21.3     | 14.9 |
| 21          | 1.01      | 0.115 | 18.34                 | 33.99              | —        | —    | —        | —    |
| 22          | 0.99      | 0.112 | 18.01                 | 33.95              | —        | —    | 19.4     | 13.5 |
| 23          | 0.97      | 0.110 | 17.69                 | 33.90              | —        | —    | —        | —    |
| 24          | 0.95      | 0.107 | 17.38                 | 33.86              | 639      | 48.2 | 17.7     | 12.3 |
| 25          | 0.93      | 0.105 | 17.08                 | 33.82              | —        | —    | —        | —    |
| 26          | 0.91      | 0.102 | 16.79                 | 33.77              | —        | —    | 16.3     | 11.3 |
| 27          | 0.89      | 0.100 | 16.50                 | 33.73              | —        | —    | —        | —    |
| 28          | 0.87      | 0.098 | 16.21                 | 33.68              | 586      | 44.0 | 15.0     | 10.3 |
| 29          | 0.85      | 0.095 | 15.92                 | 33.64              | —        | —    | —        | —    |
| 30          | 0.84      | 0.094 | 15.64                 | 33.60              | 530      | 41.0 | 13.8     | 9.5  |
| 35          | —         | —     | —                     | —                  | —        | —    | —        | —    |
| 40          | —         | —     | 14.18                 | —                  | 400      | 31.6 | 9.4      | 6.3  |
| 45          | —         | —     | —                     | —                  | —        | —    | —        | —    |
| 50          | —         | —     | 12.97                 | —                  | 290      | 23.5 | 6.5      | 4.1  |
| 60          | —         | —     | 12.16                 | —                  | 200      | 16.8 | 4.9      | 2.9  |
| 70          | —         | —     | —                     | —                  | —        | 11.1 | 3.8      | 1.9  |
| 80          | —         | —     | 11.26                 | —                  | —        | 6.5  | 3.0      | 1.2  |
| 90          | —         | —     | —                     | —                  | —        | 3.0  | —        | —    |
| 100         | —         | —     | 11.05                 | —                  | —        | 0.0  | —        | —    |

\* Free from NH<sub>3</sub> and CO<sub>2</sub>; total pressure of air + water vapor is 760 mm.



**TABLE 5.1** Solubility of Gases in Water (*Continued*)

| Temp.<br>°C | Carbon dioxide |         | Carbon monoxide |           | Chlorine |         | Ethane   |          | Ethylene |         | Hydrogen |             |
|-------------|----------------|---------|-----------------|-----------|----------|---------|----------|----------|----------|---------|----------|-------------|
|             | $\alpha$       | q       | $\alpha$        | q         | l        | q       | $\alpha$ | q        | $\alpha$ | q       | $\alpha$ | q           |
| 0           | 1.713          | 0.334 6 | 0.035 37        | 0.004 397 | —        | —       | 0.098 74 | 0.013 17 | 0.226    | 0.028 1 | 0.021 48 | 0.000 192 2 |
| 1           | 1.646          | 0.321 3 | 0.034 55        | 0.004 293 | —        | —       | 0.094 76 | 0.012 63 | 0.219    | 0.027 2 | 0.021 26 | 0.000 190 1 |
| 2           | 1.584          | 0.309 1 | 0.033 75        | 0.004 191 | —        | —       | 0.090 93 | 0.012 12 | 0.211    | 0.026 2 | 0.021 05 | 0.000 188 1 |
| 3           | 1.527          | 0.297 8 | 0.032 97        | 0.004 092 | —        | —       | 0.087 25 | 0.011 62 | 0.204    | 0.025 3 | 0.020 84 | 0.000 186 2 |
| 4           | 1.473          | 0.287 1 | 0.032 22        | 0.003 996 | —        | —       | 0.083 72 | 0.011 14 | 0.197    | 0.024 4 | 0.020 64 | 0.000 184 3 |
| 5           | 1.424          | 0.277 4 | 0.031 49        | 0.003 903 | —        | —       | 0.080 33 | 0.010 69 | 0.191    | 0.023 7 | 0.020 44 | 0.000 182 4 |
| 6           | 1.377          | 0.268 1 | 0.030 78        | 0.003 813 | —        | —       | 0.077 09 | 0.010 25 | 0.184    | 0.022 8 | 0.020 25 | 0.000 180 6 |
| 7           | 1.331          | 0.258 9 | 0.030 09        | 0.003 725 | —        | —       | 0.074 00 | 0.009 83 | 0.178    | 0.022 0 | 0.020 07 | 0.000 178 9 |
| 8           | 1.282          | 0.249 2 | 0.029 42        | 0.003 640 | —        | —       | 0.071 06 | 0.009 43 | 0.173    | 0.021 4 | 0.019 89 | 0.000 177 2 |
| 9           | 1.237          | 0.240 3 | 0.028 78        | 0.003 559 | —        | —       | 0.068 26 | 0.009 06 | 0.167    | 0.020 7 | 0.019 72 | 0.000 175 6 |
| 10          | 1.194          | 0.231 8 | 0.028 16        | 0.003 479 | 3.148    | 0.997 2 | 0.065 61 | 0.008 70 | 0.162    | 0.020 0 | 0.019 55 | 0.000 174 0 |
| 11          | 1.154          | 0.223 9 | 0.027 57        | 0.003 405 | 3.047    | 0.965 4 | 0.063 28 | 0.008 38 | 0.157    | 0.019 4 | 0.019 40 | 0.000 172 5 |
| 12          | 1.117          | 0.216 5 | 0.027 01        | 0.003 332 | 2.950    | 0.934 6 | 0.061 06 | 0.008 08 | 0.152    | 0.018 8 | 0.019 25 | 0.000 171 0 |
| 13          | 1.083          | 0.209 8 | 0.026 46        | 0.003 261 | 2.856    | 0.905 0 | 0.058 94 | 0.007 80 | 0.148    | 0.018 3 | 0.019 11 | 0.000 169 6 |
| 14          | 1.050          | 0.203 2 | 0.025 93        | 0.003 194 | 2.767    | 0.876 8 | 0.056 94 | 0.007 53 | 0.143    | 0.017 6 | 0.018 97 | 0.000 168 2 |
| 15          | 1.019          | 0.197 0 | 0.025 43        | 0.003 130 | 2.680    | 0.849 5 | 0.055 04 | 0.007 27 | 0.139    | 0.017 1 | 0.018 83 | 0.000 166 8 |
| 16          | 0.985          | 0.190 3 | 0.024 94        | 0.003 066 | 2.597    | 0.823 2 | 0.053 26 | 0.007 03 | 0.136    | 0.016 7 | 0.018 69 | 0.000 165 4 |
| 17          | 0.956          | 0.184 5 | 0.024 48        | 0.003 007 | 2.517    | 0.797 9 | 0.051 59 | 0.006 80 | 0.132    | 0.016 2 | 0.018 56 | 0.000 164 1 |
| 18          | 0.928          | 0.178 9 | 0.024 02        | 0.002 947 | 2.440    | 0.773 8 | 0.050 03 | 0.006 59 | 0.129    | 0.015 8 | 0.018 44 | 0.000 162 8 |
| 19          | 0.902          | 0.173 7 | 0.023 60        | 0.002 891 | 2.368    | 0.751 0 | 0.048 58 | 0.006 39 | 0.125    | 0.015 3 | 0.018 31 | 0.000 161 6 |

**TABLE 5.1** Solubility of Gases in Water (*Continued*)

| Temp.<br>°C | Carbon dioxide |         | Carbon monoxide |           | Chlorine |         | Ethane   |          | Ethylene |         | Hydrogen |             |
|-------------|----------------|---------|-----------------|-----------|----------|---------|----------|----------|----------|---------|----------|-------------|
|             | α              | q       | α               | q         | l        | q       | α        | q        | α        | q       | α        | q           |
| 20          | 0.878          | 0.168 8 | 0.023 19        | 0.002 838 | 2.299    | 0.729 3 | 0.047 24 | 0.006 20 | 0.122    | 0.014 9 | 0.018 19 | 0.000 160 3 |
| 21          | 0.854          | 0.164 0 | 0.022 81        | 0.002 789 | 2.238    | 0.710 0 | 0.045 89 | 0.006 02 | 0.119    | 0.014 6 | 0.018 05 | 0.000 158 8 |
| 22          | 0.829          | 0.159 0 | 0.022 44        | 0.002 739 | 2.180    | 0.691 8 | 0.044 59 | 0.005 84 | 0.116    | 0.014 2 | 0.017 92 | 0.000 157 5 |
| 23          | 0.804          | 0.154 0 | 0.022 08        | 0.002 691 | 2.123    | 0.673 9 | 0.043 35 | 0.005 67 | 0.114    | 0.013 9 | 0.017 79 | 0.000 156 1 |
| 24          | 0.781          | 0.149 3 | 0.021 74        | 0.002 646 | 2.070    | 0.657 2 | 0.042 17 | 0.005 51 | 0.111    | 0.013 5 | 0.017 66 | 0.000 154 8 |
| 25          | 0.759          | 0.144 9 | 0.021 42        | 0.002 603 | 2.019    | 0.641 3 | 0.041 04 | 0.005 35 | 0.108    | 0.013 1 | 0.017 54 | 0.000 153 5 |
| 26          | 0.738          | 0.140 6 | 0.021 10        | 0.002 560 | 1.970    | 0.625 9 | 0.039 97 | 0.005 20 | 0.106    | 0.012 9 | 0.017 42 | 0.000 152 2 |
| 27          | 0.718          | 0.136 6 | 0.020 80        | 0.002 519 | 1.923    | 0.611 2 | 0.038 95 | 0.005 06 | 0.104    | 0.012 6 | 0.017 31 | 0.000 150 9 |
| 28          | 0.699          | 0.132 7 | 0.020 51        | 0.002 479 | 1.880    | 0.597 5 | 0.037 99 | 0.004 93 | 0.102    | 0.012 3 | 0.017 20 | 0.000 149 6 |
| 29          | 0.682          | 0.129 2 | 0.020 24        | 0.002 442 | 1.839    | 0.584 7 | 0.037 09 | 0.004 80 | 0.100    | 0.012 1 | 0.017 09 | 0.000 148 4 |
| 30          | 0.665          | 0.125 7 | 0.019 98        | 0.002 405 | 1.799    | 0.572 3 | 0.036 24 | 0.004 68 | 0.098    | 0.011 8 | 0.016 99 | 0.000 147 4 |
| 35          | 0.592          | 0.110 5 | 0.018 77        | 0.002 231 | 1.602    | 0.510 4 | 0.032 30 | 0.004 12 | —        | —       | 0.016 66 | 0.000 142 5 |
| 40          | 0.530          | 0.097 3 | 0.017 75        | 0.002 075 | 1.438    | 0.459 0 | 0.029 15 | 0.003 66 | —        | —       | 0.016 44 | 0.000 138 4 |
| 45          | 0.479          | 0.086 0 | 0.016 90        | 0.001 933 | 1.322    | 0.422 8 | 0.026 60 | 0.003 27 | —        | —       | 0.016 24 | 0.000 134 1 |
| 50          | 0.436          | 0.076 1 | 0.016 15        | 0.001 797 | 1.225    | 0.392 5 | 0.024 59 | 0.002 94 | —        | —       | 0.016 08 | 0.000 128 7 |
| 60          | 0.359          | 0.057 6 | 0.014 88        | 0.001 522 | 1.023    | 0.329 5 | 0.021 77 | 0.002 39 | —        | —       | 0.016 00 | 0.000 117 8 |
| 70          | —              | —       | 0.014 40        | 0.001 276 | 0.862    | 0.279 3 | 0.019 48 | 0.001 85 | —        | —       | 0.016 0  | 0.000 102   |
| 80          | —              | —       | 0.014 30        | 0.000 980 | 0.683    | 0.222 7 | 0.018 26 | 0.001 34 | —        | —       | 0.016 0  | 0.000 079   |
| 90          | —              | —       | 0.014 2         | 0.000 57  | 0.39     | 0.127   | 0.017 6  | 0.000 8  | —        | —       | 0.016 0  | 0.000 046   |
| 100         | —              | —       | 0.014 1         | 0.000 00  | 0.00     | 0.000   | 0.017 2  | 0.000 0  | —        | —       | 0.016 0  | 0.000 000   |

**TABLE 5.1** Solubility of Gases in Water (*Continued*)

| Temp.<br>°C | Hydrogen sulfide |         | Methane  |           | Nitric oxide |           | Nitrogen* |           | Oxygen   |           | Sulfur dioxide |       |
|-------------|------------------|---------|----------|-----------|--------------|-----------|-----------|-----------|----------|-----------|----------------|-------|
|             | α                | q       | α        | q         | α            | q         | α         | q         | α        | q         | l              | q     |
| 0           | 4.670            | 0.706 6 | 0.055 63 | 0.003 959 | 0.073 81     | 0.009 833 | 0.023 54  | 0.002 942 | 0.048 89 | 0.006 945 | 79.789         | 22.83 |
| 1           | 4.522            | 0.683 9 | 0.054 01 | 0.003 842 | 0.071 84     | 0.009 564 | 0.022 97  | 0.002 869 | 0.047 58 | 0.006 756 | 77.210         | 22.09 |
| 2           | 4.379            | 0.661 9 | 0.052 44 | 0.003 728 | 0.069 93     | 0.009 305 | 0.022 41  | 0.002 798 | 0.046 33 | 0.006 574 | 74.691         | 21.37 |
| 3           | 4.241            | 0.640 7 | 0.050 93 | 0.003 619 | 0.068 09     | 0.009 057 | 0.021 87  | 0.002 730 | 0.045 12 | 0.006 400 | 72.230         | 20.66 |
| 4           | 4.107            | 0.620 1 | 0.049 46 | 0.003 513 | 0.066 32     | 0.008 816 | 0.021 35  | 0.002 663 | 0.043 97 | 0.006 232 | 69.828         | 19.98 |
| 5           | 3.977            | 0.600 1 | 0.048 05 | 0.003 410 | 0.064 61     | 0.008 584 | 0.020 86  | 0.002 600 | 0.042 87 | 0.006 072 | 67.485         | 19.31 |
| 6           | 3.852            | 0.580 9 | 0.046 69 | 0.003 312 | 0.062 98     | 0.008 361 | 0.020 37  | 0.002 537 | 0.041 80 | 0.005 918 | 65.200         | 18.65 |
| 7           | 3.732            | 0.562 4 | 0.045 39 | 0.003 217 | 0.061 40     | 0.008 147 | 0.019 90  | 0.002 477 | 0.040 80 | 0.005 773 | 62.973         | 18.02 |
| 8           | 3.616            | 0.544 6 | 0.044 13 | 0.003 127 | 0.059 90     | 0.007 943 | 0.019 45  | 0.002 419 | 0.039 83 | 0.005 632 | 60.805         | 17.40 |
| 9           | 3.505            | 0.527 6 | 0.042 92 | 0.003 039 | 0.058 46     | 0.007 747 | 0.019 02  | 0.002 365 | 0.038 91 | 0.005 498 | 58.697         | 16.80 |
| 10          | 3.399            | 0.511 2 | 0.041 77 | 0.002 955 | 0.057 09     | 0.007 560 | 0.018 61  | 0.002 312 | 0.038 02 | 0.005 368 | 56.647         | 16.21 |
| 11          | 3.300            | 0.496 0 | 0.040 72 | 0.002 879 | 0.055 87     | 0.007 393 | 0.018 23  | 0.002 263 | 0.037 18 | 0.005 246 | 54.655         | 15.64 |
| 12          | 3.206            | 0.481 4 | 0.039 70 | 0.002 805 | 0.054 70     | 0.007 233 | 0.017 86  | 0.002 216 | 0.036 37 | 0.005 128 | 52.723         | 15.09 |
| 13          | 3.115            | 0.467 4 | 0.038 72 | 0.002 733 | 0.053 57     | 0.007 078 | 0.017 50  | 0.002 170 | 0.035 59 | 0.005 014 | 50.849         | 14.56 |
| 14          | 3.028            | 0.454 0 | 0.037 79 | 0.002 665 | 0.052 50     | 0.006 930 | 0.017 17  | 0.002 126 | 0.034 86 | 0.004 906 | 49.033         | 14.04 |
| 15          | 2.945            | 0.441 1 | 0.036 90 | 0.002 599 | 0.051 47     | 0.006 788 | 0.016 85  | 0.002 085 | 0.034 15 | 0.004 802 | 47.276         | 13.54 |
| 16          | 2.865            | 0.428 7 | 0.036 06 | 0.002 538 | 0.050 49     | 0.006 652 | 0.016 54  | 0.002 045 | 0.033 48 | 0.004 703 | 45.578         | 13.05 |
| 17          | 2.789            | 0.416 9 | 0.035 25 | 0.002 478 | 0.049 56     | 0.006 524 | 0.016 25  | 0.002 006 | 0.032 83 | 0.004 606 | 43.939         | 12.59 |
| 18          | 2.717            | 0.405 6 | 0.034 48 | 0.002 422 | 0.048 68     | 0.006 400 | 0.015 97  | 0.001 970 | 0.032 20 | 0.004 514 | 42.360         | 12.14 |
| 19          | 2.647            | 0.394 8 | 0.033 76 | 0.002 369 | 0.047 85     | 0.006 283 | 0.015 70  | 0.001 935 | 0.031 61 | 0.004 426 | 40.838         | 11.70 |

**TABLE 5.1** Solubility of Gases in Water (*Continued*)

| Temp.<br>°C | Hydrogen sulfide |         | Methane  |           | Nitric oxide |           | Nitrogen* |           | Oxygen   |           | Sulfur dioxide |       |
|-------------|------------------|---------|----------|-----------|--------------|-----------|-----------|-----------|----------|-----------|----------------|-------|
|             | α                | q       | α        | q         | α            | q         | α         | q         | α        | q         | l              | q     |
| 20          | 2.582            | 0.384 6 | 0.033 08 | 0.002 319 | 0.047 06     | 0.006 173 | 0.015 45  | 0.001 901 | 0.031 02 | 0.004 339 | 39.374         | 11.28 |
| 21          | 2.517            | 0.374 5 | 0.032 43 | 0.002 270 | 0.046 25     | 0.006 059 | 0.015 22  | 0.001 869 | 0.030 44 | 0.004 252 | 37.970         | 10.88 |
| 22          | 2.456            | 0.364 8 | 0.031 80 | 0.002 222 | 0.045 45     | 0.005 947 | 0.014 98  | 0.001 838 | 0.029 88 | 0.004 169 | 36.617         | 10.50 |
| 23          | 2.396            | 0.355 4 | 0.031 19 | 0.002 177 | 0.044 69     | 0.005 838 | 0.014 75  | 0.001 809 | 0.029 34 | 0.004 087 | 35.302         | 10.12 |
| 24          | 2.338            | 0.346 3 | 0.030 61 | 0.002 133 | 0.043 95     | 0.005 733 | 0.014 54  | 0.001 780 | 0.028 81 | 0.004 007 | 34.026         | 9.76  |
| 25          | 2.282            | 0.337 5 | 0.030 06 | 0.002 091 | 0.043 23     | 0.005 630 | 0.014 34  | 0.001 751 | 0.028 31 | 0.003 931 | 32.786         | 9.41  |
| 26          | 2.229            | 0.329 0 | 0.029 52 | 0.002 050 | 0.042 54     | 0.005 530 | 0.014 13  | 0.001 724 | 0.027 83 | 0.003 857 | 31.584         | 9.06  |
| 27          | 2.177            | 0.320 8 | 0.029 01 | 0.002 011 | 0.041 88     | 0.005 435 | 0.013 94  | 0.001 698 | 0.027 36 | 0.003 787 | 30.422         | 8.73  |
| 28          | 2.128            | 0.313 0 | 0.028 52 | 0.001 974 | 0.041 24     | 0.005 342 | 0.013 76  | 0.001 672 | 0.026 91 | 0.003 718 | 29.314         | 8.42  |
| 29          | 2.081            | 0.305 5 | 0.028 06 | 0.001 938 | 0.040 63     | 0.005 252 | 0.013 58  | 0.001 647 | 0.026 49 | 0.003 651 | 28.210         | 8.10  |
| 30          | 2.037            | 0.298 3 | 0.027 62 | 0.001 904 | 0.040 04     | 0.005 165 | 0.013 42  | 0.001 624 | 0.026 08 | 0.003 588 | 27.161         | 7.80  |
| 35          | 1.831            | 0.264 8 | 0.025 46 | 0.001 733 | 0.037 34     | 0.004 757 | 0.012 56  | 0.001 501 | 0.024 40 | 0.003 315 | 22.489         | 6.47  |
| 40          | 1.660            | 0.236 1 | 0.023 69 | 0.001 586 | 0.035 07     | 0.004 394 | 0.011 84  | 0.001 391 | 0.023 06 | 0.003 082 | 18.766         | 5.41  |
| 45          | 1.516            | 0.211 0 | 0.022 38 | 0.001 466 | 0.033 11     | 0.004 059 | 0.011 30  | 0.001 300 | 0.021 87 | 0.002 858 | —              | —     |
| 50          | 1.392            | 0.188 3 | 0.021 34 | 0.001 359 | 0.031 52     | 0.003 758 | 0.010 88  | 0.001 216 | 0.020 90 | 0.002 657 | —              | —     |
| 60          | 1.190            | 0.148 0 | 0.019 54 | 0.001 144 | 0.029 54     | 0.003 237 | 0.010 23  | 0.001 052 | 0.019 46 | 0.002 274 | —              | —     |
| 70          | 1.022            | 0.110 1 | 0.018 25 | 0.000 926 | 0.028 10     | 0.002 668 | 0.009 77  | 0.000 851 | 0.018 33 | 0.001 856 | —              | —     |
| 80          | 0.917            | 0.076 5 | 0.017 70 | 0.000 695 | 0.027 00     | 0.001 984 | 0.009 58  | 0.000 660 | 0.017 61 | 0.001 381 | —              | —     |
| 90          | 0.84             | 0.041   | 0.017 35 | 0.000 40  | 0.026 5      | 0.001 13  | 0.009 5   | 0.000 38  | 0.017 2  | 0.000 79  | —              | —     |
| 100         | 0.81             | 0.000   | 0.017 0  | 0.000 00  | 0.026 3      | 0.000 00  | 0.009 5   | 0.000 00  | 0.017 0  | 0.000 00  | —              | —     |

\* Atmospheric nitrogen containing 98.815% N<sub>2</sub> by volume + 1.185% inert gases.

**TABLE 5.1** Solubility of Gases in Water (*Continued*)

| Substance         |                                | 0°      | 10°                    | 20°                    | 30°                   | 40°                     | 60°                | 80°                     |
|-------------------|--------------------------------|---------|------------------------|------------------------|-----------------------|-------------------------|--------------------|-------------------------|
| Argon             | $\alpha$                       | 0.052 8 | 0.041 3                | 0.033 7                | 0.028 8               | 0.025 1                 | 0.020 9            | 0.018 4                 |
| Helium            | A                              | 0.009 8 | 0.009 11               | 0.008 6                | 0.008 39              | 0.008 41                | 0.009 02           | 0.009 42 <sup>70°</sup> |
| Hydrogen bromide  | l                              | 612     | 582                    |                        | 533 <sup>25°</sup>    |                         | 469 <sup>50°</sup> | 406 <sup>75°</sup>      |
| Hydrogen chloride | $\alpha$                       | 512     | 475                    | 442                    | 412                   | 385                     | 339                |                         |
| Krypton           | $\alpha$                       | 0.110 5 | 0.081 0                | 0.062 6                | 0.051 1               | 0.043 3                 | 0.035 7            |                         |
| Neon              | A                              |         | 0.011 7 <sup>9°</sup>  | 0.010 6                | 0.010 0               | 0.009 48 <sup>42°</sup> |                    | 0.009 84 <sup>73°</sup> |
| Nitrous oxide     | A                              |         | 0.88                   | 0.63                   |                       |                         |                    |                         |
| Ozone             | $\text{g} \cdot \text{L}^{-1}$ | 0.039 4 | 0.029 9 <sup>12°</sup> | 0.021 0 <sup>19°</sup> | 0.0139 <sup>27°</sup> | 0.004 2                 | 0                  |                         |
| Radon             | $\alpha$                       | 0.510   | 0.326                  | 0.222                  | 0.162                 | 0.126                   | 0.085              |                         |
| Xenon             | $\alpha$                       | 0.242   | 0.174                  | 0.123                  | 0.098                 | 0.082                   |                    |                         |

**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures

Solubilities are expressed as the number of grams of substance of stated molecular formula which when dissolved in 100 g of water make a saturated solution at the temperature stated (°C).

| Substance                        | Formula                                                           | 0°    | 10°   | 20°   | 30°   | 40°   | 60°   | 80°  | 90°  | 100° |
|----------------------------------|-------------------------------------------------------------------|-------|-------|-------|-------|-------|-------|------|------|------|
| <b>Aluminum</b> chloride         | AlCl <sub>3</sub>                                                 | 43.9  | 44.9  | 45.8  | 46.6  | 47.3  | 48.1  | 48.6 |      | 49.0 |
| fluoride                         | AlF <sub>3</sub>                                                  | 0.56  | 0.56  | 0.67  | 0.78  | 0.91  | 1.1   | 1.32 |      | 1.72 |
| nitrate                          | Al(NO <sub>3</sub> ) <sub>3</sub>                                 | 60.0  | 66.7  | 73.9  | 81.8  | 88.7  | 106   | 132  | 153  | 160  |
| perchlorate                      | Al(ClO <sub>4</sub> ) <sub>3</sub>                                | 122   | 128   | 133   |       |       |       |      |      | 182  |
| sulfate                          | Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                   | 31.2  | 33.5  | 36.4  | 40.4  | 45.8  | 59.2  | 73.0 | 80.8 | 89.0 |
| thallium(I) sulfate              | Al <sub>2</sub> Tl <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub>   | 3.15  | 4.60  | 6.39  | 9.37  | 14.39 | 35.35 |      |      |      |
| <b>Ammonium</b> aluminum sulfate | NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub>                 | 2.10  | 5.00  | 7.74  | 10.9  | 14.9  | 26.7  |      |      |      |
| azide                            | NH <sub>4</sub> N <sub>3</sub>                                    | 16.0  |       | 25.3  |       | 37.1  |       |      |      |      |
| bromide                          | NH <sub>4</sub> Br                                                | 60.5  | 68.1  | 76.4  | 83.2  | 91.2  | 108   | 125  | 135  | 145  |
| chloride                         | NH <sub>4</sub> Cl                                                | 29.4  | 33.2  | 37.2  | 41.4  | 45.8  | 55.3  | 65.6 | 71.2 | 77.3 |
| chloroiridate(IV)                | (NH <sub>4</sub> ) <sub>2</sub> IrCl <sub>6</sub>                 | 0.56  | 0.71  | 0.95  | 1.20  | 1.56  | 2.45  | 4.38 |      |      |
| chloroplatinate(IV)              | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub>                 | 0.289 | 0.374 | 0.499 | 0.637 | 0.815 | 1.44  | 2.16 | 2.61 | 3.36 |
| chromate                         | (NH <sub>4</sub> ) <sub>2</sub> CrO <sub>4</sub>                  | 25.0  | 29.2  | 34.0  | 39.3  | 45.3  | 59.0  | 76.1 |      |      |
| chromium(III) sulfate            | (NH <sub>4</sub> )Cr(SO <sub>4</sub> ) <sub>2</sub>               | 3.95  |       |       | 18.8  | 32.6  |       |      |      |      |
| cobalt(II) sulfate               | (NH <sub>4</sub> ) <sub>2</sub> Co(SO <sub>4</sub> ) <sub>2</sub> | 6.0   | 9.5   | 13.0  | 17.0  | 22.0  | 33.5  | 49.0 | 58.0 | 75.1 |
| dichromate                       | (NH <sub>4</sub> ) <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>    | 18.2  | 25.5  | 35.6  | 46.5  | 58.5  | 86.0  | 115  |      | 156  |
| dihydrogen arsenate              | NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>                   | 33.7  |       | 48.7  |       | 63.8  | 83.0  | 107  | 122  |      |
| dihydrogen phosphate             | NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>                    | 22.7  | 29.5  | 37.4  | 46.4  | 56.7  | 82.5  | 118  |      | 173  |
| dithionate                       | (NH <sub>4</sub> ) <sub>2</sub> S <sub>2</sub> O <sub>6</sub>     | 133   | 151   | 166   | 179   |       |       |      |      |      |
| formate                          | NH <sub>4</sub> CHO <sub>2</sub>                                  | 102   |       | 143   |       | 204   | 311   | 533  |      |      |
| hydrogen carbonate               | NH <sub>4</sub> HCO <sub>3</sub>                                  | 11.9  | 16.1  | 21.7  | 28.4  | 36.6  | 59.2  | 109  | 170  | 354  |
| hydrogen phosphate               | (NH <sub>4</sub> ) <sub>2</sub> HPO <sub>4</sub>                  | 42.9  | 62.9  | 68.9  | 75.1  | 81.8  | 97.2  |      |      |      |
| hydrogen tartrate                | NH <sub>4</sub> C <sub>4</sub> H <sub>5</sub> O <sub>6</sub>      | 1.00  | 1.88  | 2.70  |       |       |       |      |      |      |
| iodide                           | NH <sub>4</sub> I                                                 | 155   | 163   | 172   | 182   | 191   | 209   | 229  |      | 250  |
| iron(II) sulfate                 | (NH <sub>4</sub> ) <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> | 12.5  | 17.2  | 26.4  | 33    | 46    |       |      |      |      |

**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                           | Formula                                                                               | 0°    | 10°   | 20°                 | 30°   | 40°  | 60°                          | 80°   | 90°   | 100°                |
|-------------------------------------|---------------------------------------------------------------------------------------|-------|-------|---------------------|-------|------|------------------------------|-------|-------|---------------------|
| <b>Ammonium</b> magnesium sulfate   | (NH <sub>4</sub> ) <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub>                     | 11.8  | 14.6  | 18.0                | 21.7  | 25.8 | 35.1                         | 48.3  |       | 65.7                |
| nickel sulfate                      | (NH <sub>4</sub> ) <sub>2</sub> Ni(SO <sub>4</sub> ) <sub>2</sub>                     | 1.00  | 4.00  | 6.50                | 9.20  | 12.0 | 17.0                         |       |       |                     |
| nitrate                             | NH <sub>4</sub> NO <sub>3</sub>                                                       | 118   | 150   | 192                 | 242   | 297  | 421                          | 580   | 740   | 871                 |
| oxalate                             | (NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                         | 2.2   | 3.21  | 4.45                | 6.09  | 8.18 | 14.0                         | 22.4  | 27.9  | 34.7                |
| perchlorate                         | NH <sub>4</sub> ClO <sub>4</sub>                                                      | 12.0  | 16.4  | 21.7                | 27.7  | 34.6 | 49.9                         | 68.9  |       |                     |
| selenite                            | (NH <sub>4</sub> ) <sub>2</sub> SeO <sub>3</sub>                                      | 96    | 105   | 115                 | 126   | 143  | 192                          |       |       |                     |
| sulfate                             | (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>                                       | 70.6  | 73.0  | 75.4                | 78.0  | 81   | 88                           | 95    |       | 103                 |
| sulfite                             | (NH <sub>4</sub> ) <sub>2</sub> SO <sub>3</sub>                                       | 47.9  | 54.0  | 60.8                | 68.8  | 78.4 | 104                          | 144   | 150   | 153                 |
| tartrate                            | (NH <sub>4</sub> ) <sub>2</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub>          | 45.0  | 55.0  | 63.0                | 70.5  | 76.5 | 86.9                         |       |       |                     |
| thioantimonate(V)                   | (NH <sub>4</sub> ) <sub>3</sub> SbS <sub>4</sub>                                      | 71.2  |       | 91.2                | 120   |      |                              |       |       |                     |
| thiocyanate                         | NH <sub>4</sub> SCN                                                                   | 120   | 144   | 170                 | 208   | 234  | 346                          |       |       |                     |
| vanadate                            | NH <sub>4</sub> VO <sub>3</sub>                                                       |       |       | 0.48                | 0.84  | 1.32 | 2.42                         |       |       |                     |
| zinc sulfate                        | (NH <sub>4</sub> ) <sub>2</sub> Zn(SO <sub>4</sub> ) <sub>2</sub>                     | 7.0   | 9.5   | 12.5                | 16.0  | 20.0 | 30.0                         | 46.6  | 58.0  | 72.4                |
| <b>Antimony(III)</b> chloride       | SbCl <sub>3</sub>                                                                     | 602   |       | 910                 | 1087  | 1368 | [completely miscible at 72°] |       |       |                     |
| fluoride                            | SbF <sub>3</sub>                                                                      | 385   |       | 444                 | 562   |      |                              |       |       |                     |
| <b>Arsenic</b> hydride (760 mm), cc | AsH <sub>3</sub>                                                                      | 42    | 30    | 28                  |       |      |                              |       |       |                     |
| oxide (pent-)                       | As <sub>2</sub> O <sub>5</sub>                                                        | 59.5  | 62.1  | 65.8                | 69.8  | 71.2 | 73.0                         | 75.1  |       | 76.7                |
| oxide (tri-)                        | As <sub>2</sub> O <sub>3</sub>                                                        | 1.20  | 1.49  | 1.82                | 2.31  | 2.93 | 4.31                         | 6.11  |       | 8.2                 |
| <b>Barium</b> acetate               | Ba(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> · 3H <sub>2</sub> O    | 58.8  | 62    | 72                  | 75    | 78.5 | 75.0                         | 74.0  |       | 74.8                |
| azide                               | Ba(N <sub>3</sub> ) <sub>2</sub>                                                      | 12.5  | 16.1  | 17.4 <sup>17°</sup> |       |      |                              |       |       |                     |
| bromate                             | Ba(BrO <sub>3</sub> ) <sub>2</sub> · H <sub>2</sub> O                                 | 0.29  | 0.44  | 0.65                | 0.95  | 1.31 | 2.27                         | 3.52  | 4.26  | 5.39                |
| bromide                             | BaBr <sub>2</sub> · 2H <sub>2</sub> O                                                 | 98    | 101   | 104                 | 109   | 114  | 123                          | 135   |       | 149                 |
| <i>n</i> -butyrate                  | Ba(C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub>                        | 37.0  | 36.1  | 35.4                | 34.9  | 35.2 | 37.2                         | 41.7  | 45.5  | 48.1 <sup>95°</sup> |
| caproate                            | Ba(C <sub>6</sub> H <sub>11</sub> O <sub>2</sub> ) <sub>2</sub> · 3.5H <sub>2</sub> O | 11.71 | 8.38  | 6.89                | 5.87  | 5.79 | 8.39                         | 14.71 | 19.28 |                     |
| chlorate                            | Ba(ClO <sub>3</sub> ) <sub>2</sub> · H <sub>2</sub> O                                 | 20.3  | 26.9  | 33.9                | 41.6  | 49.7 | 66.7                         | 84.8  |       | 105                 |
| chloride                            | BaCl <sub>2</sub> · 2H <sub>2</sub> O                                                 | 31.2  | 33.5  | 35.8                | 38.1  | 40.8 | 46.2                         | 52.5  | 55.8  | 59.4                |
| chlorite                            | Ba(ClO <sub>2</sub> ) <sub>2</sub>                                                    | 43.9  | 44.6  | 45.4                |       | 47.9 | 53.8                         | 66.6  |       | 80.8                |
| fluoride                            | BaF <sub>2</sub>                                                                      |       | 0.159 | 0.160               | 0.162 |      |                              |       |       |                     |

|                          |                                                                                      |       |       |       |                    |       |       |       |       |                     |
|--------------------------|--------------------------------------------------------------------------------------|-------|-------|-------|--------------------|-------|-------|-------|-------|---------------------|
| formate                  | Ba(CHO <sub>2</sub> ) <sub>2</sub>                                                   | 26.2  | 28.0  | 29.9  | 31.9               | 34.0  | 38.6  | 44.2  | 47.6  | 51.3                |
| hydroxide                | Ba(OH) <sub>2</sub>                                                                  | 1.67  | 2.48  | 3.89  | 5.59               | 8.22  | 20.94 | 101.4 |       |                     |
| iodate                   | Ba(IO <sub>3</sub> ) <sub>2</sub>                                                    |       |       | 0.035 | 0.046              | 0.057 |       |       |       |                     |
| iodide                   | BaI <sub>2</sub> · 2H <sub>2</sub> O                                                 | 182   | 201   | 223   | 250                |       | 264   |       | 291   | 301                 |
| nitrate                  | Ba(NO <sub>3</sub> ) <sub>2</sub>                                                    | 4.95  | 6.67  | 9.02  | 11.48              | 14.1  | 20.4  | 27.2  |       | 34.4                |
| nitrite                  | Ba(NO <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O                                 | 50.3  | 60    | 72.8  |                    | 102   | 151   | 222   | 261   | 325                 |
| perchlorate              | Ba(ClO <sub>4</sub> ) <sub>2</sub> · 3H <sub>2</sub> O                               | 239   |       | 336   |                    | 416   | 495   | 575   |       | 653                 |
| propionate               | Ba(C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O    | 57.2  | 56.8  |       | 57.5               | 59.0  | 62.0  | 67.8  | 73.0  | 82.7                |
| isosuccinate             | BaC <sub>4</sub> H <sub>4</sub> O <sub>4</sub>                                       | 0.421 | 0.432 | 0.418 | 0.393              | 0.366 | 0.306 | 0.237 |       |                     |
| sulfamate                | Ba(SO <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub>                                    | 18.3  | 22.3  | 26.8  | 32.5               | 38.5  | 49.6  | 61.5  |       | 73.5                |
| sulfide                  | BaS                                                                                  | 2.88  | 4.89  | 7.86  | 10.38              | 14.89 | 27.69 | 49.91 | 67.34 | 60.29               |
| tartrate                 | Ba(C <sub>2</sub> H <sub>2</sub> O <sub>3</sub> ) <sub>2</sub>                       | 0.021 | 0.024 | 0.028 | 0.032              | 0.035 | 0.044 | 0.053 |       |                     |
| <b>Beryllium</b> nitrate | Be(NO <sub>3</sub> ) <sub>2</sub>                                                    | 97    | 102   | 108   | 113                | 125   | 178   |       |       |                     |
| sulfate                  | BeSO <sub>4</sub>                                                                    | 37.0  | 37.6  | 39.1  | 41.4               | 45.8  | 53.1  | 67.2  |       | 82.8                |
| <b>Boric acid</b>        | H <sub>3</sub> BO <sub>3</sub>                                                       | 2.67  | 3.73  | 5.04  | 6.72               | 8.72  | 14.81 | 23.62 | 30.38 | 40.25               |
| <b>Cadmium</b> bromide   | CdBr <sub>2</sub>                                                                    | 56.3  | 75.4  | 98.8  | 129                | 152   | 153   | 156   |       | 160                 |
| chlorate                 | Cd(ClO <sub>3</sub> ) <sub>2</sub>                                                   | 299   | 308   | 322   | 348                | 376   | 455   |       |       |                     |
| chloride                 | CdCl <sub>2</sub> · 2.5H <sub>2</sub> O                                              | 90    | 100   | 113   | 132                |       |       |       |       |                     |
|                          | CdCl <sub>2</sub> · H <sub>2</sub> O                                                 |       | 135   | 135   | 135                | 135   | 136   | 140   |       | 147                 |
| formate                  | Cd(CHO <sub>2</sub> ) <sub>2</sub>                                                   | 8.3   | 11.1  | 14.4  | 18.6               | 25.3  | 59.5  | 80.5  | 85.2  | 94.6                |
| iodide                   | CdI <sub>2</sub>                                                                     | 78.7  |       | 84.7  | 87.9               | 92.1  | 100   | 111   |       | 125                 |
| nitrate                  | Cd(NO <sub>3</sub> ) <sub>2</sub>                                                    | 122   | 136   | 150   | 167                | 194   | 310   | 713   |       |                     |
| perchlorate              | Cd(ClO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                               |       | 180   | 188   | 195                | 203   | 221   | 243   |       | 272                 |
| selenate                 | CdSeO <sub>4</sub>                                                                   | 72.5  | 68.4  | 64.0  | 58.9               | 55.0  | 44.2  | 32.5  | 27.2  | 22.0                |
| sulfate                  | CdSO <sub>4</sub>                                                                    | 75.4  | 76.0  | 76.6  |                    | 78.5  | 81.8  | 66.7  | 63.1  | 60.8                |
| <b>Calcium</b> acetate   | Ca(OAc) <sub>2</sub> · 2H <sub>2</sub> O                                             | 37.4  | 36.0  | 34.7  | 33.8               | 33.2  | 32.7  | 33.5  | 31.1  | 29.7                |
| benzoate                 | Ca(OBz) <sub>2</sub> · 3H <sub>2</sub> O                                             | 2.32  | 2.45  | 2.72  | 3.02               | 3.42  | 4.71  | 6.87  | 8.55  | 8.70                |
| bromide                  | CaBr <sub>2</sub> · 6H <sub>2</sub> O                                                | 125   | 132   | 143   | 185 <sup>34°</sup> | 213   | 278   | 295   |       | 312 <sup>105°</sup> |
| butyrate                 | Ca(C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub>                       | 20.31 | 19.15 | 18.20 | 17.25              | 16.40 | 15.15 | 14.95 |       | 15.85               |
| cacodylate               | Ca(C <sub>2</sub> H <sub>6</sub> AsO <sub>2</sub> ) <sub>2</sub> · 9H <sub>2</sub> O | 48    | 52    | 59    | 71                 |       |       |       |       |                     |
| chloride                 | CaCl <sub>2</sub> · 6H <sub>2</sub> O                                                | 59.5  | 64.7  | 74.5  | 100                | 128   | 137   | 147   | 154   | 159                 |
| chromate                 | CaCrO <sub>4</sub>                                                                   | 4.5   |       | 2.25  | 1.83               | 1.49  | 0.83  |       |       |                     |
| (mn)                     | CaCrO <sub>4</sub> · 2H <sub>2</sub> O                                               | 17.3  |       | 16.6  | 16.1               |       |       |       |       |                     |
| formate                  | Ca(CHO <sub>2</sub> ) <sub>2</sub>                                                   | 16.15 |       | 16.60 |                    | 17.05 | 17.50 | 17.95 |       | 18.40               |
| gluconate                | Ca(C <sub>6</sub> H <sub>11</sub> O <sub>7</sub> ) <sub>2</sub> · H <sub>2</sub> O   |       |       | 3.72  |                    | 5.29  |       | 12.11 | 36.80 | 57.2 <sup>96°</sup> |
| hydrogen carbonate       | Ca(HCO <sub>3</sub> ) <sub>2</sub>                                                   | 16.15 |       | 16.60 |                    | 17.05 | 17.50 | 17.95 |       | 18.40               |
| hydroxide                | Ca(OH) <sub>2</sub>                                                                  | 0.189 | 0.182 | 0.173 | 0.160              | 0.141 | 0.121 |       | 0.086 | 0.076               |



**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                              | Formula                                                                       | 0°    | 10°   | 20°                  | 30°                 | 40°                 | 60°                  | 80°                  | 90°                 | 100°  |
|----------------------------------------|-------------------------------------------------------------------------------|-------|-------|----------------------|---------------------|---------------------|----------------------|----------------------|---------------------|-------|
| <b>Calcium</b> iodate                  | $\text{Ca}(\text{IO}_3)_2 \cdot 6\text{H}_2\text{O}$                          | 0.090 |       | 0.24                 | 0.38                | 0.52                | 0.65                 | 0.66                 | 0.67                |       |
| iodide                                 | $\text{CaI}_2$                                                                | 64.6  | 66.0  | 67.6                 | 69.0                | 70.8                | 74                   | 78                   |                     | 81    |
| lactate                                | $\text{Ca}(\text{C}_3\text{H}_5\text{O}_3)_2 \cdot 5\text{H}_2\text{O}$       | 3.1   |       | 5.4 <sup>15°</sup>   | 7.9                 |                     |                      |                      |                     |       |
| levulinate                             | $\text{Ca}(\text{C}_{10}\text{H}_{14}\text{O}_6)_2 \cdot 2\text{H}_2\text{O}$ | 38.1  |       | 45.1 <sup>16°</sup>  | 55.0                | 70.3 <sup>45°</sup> | 88.7 <sup>55°</sup>  |                      |                     |       |
| malonate                               | $\text{Ca}(\text{C}_3\text{H}_2\text{O}_4)_2$                                 | 0.29  | 0.33  | 0.36                 | 0.40                | 0.42                | 0.46                 | 0.48                 |                     |       |
| nitrate                                | $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$                          | 102   | 115   | 129                  | 152                 | 191                 |                      | 358                  |                     | 363   |
| nitrite                                | $\text{Ca}(\text{NO}_2)_2 \cdot 4\text{H}_2\text{O}$                          | 63.9  |       | 84.5 <sup>18°</sup>  | 104                 |                     | 134                  | 151                  | 166                 | 178   |
| propionate                             | $\text{Ca}(\text{C}_3\text{H}_5\text{O}_2)_2 \cdot \text{H}_2\text{O}$        | 42.80 |       | 39.85                |                     |                     | 38.25                | 39.85                | 42.15               | 48.44 |
| selenate                               | $\text{CaSeO}_4 \cdot 2\text{H}_2\text{O}$                                    | 9.73  | 9.77  | 9.22                 | 8.79                | 7.14                |                      |                      |                     |       |
| succinate                              | $\text{Ca}(\text{C}_3\text{H}_2\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$       | 1.127 | 1.22  | 1.28                 |                     | 1.18                | 0.89                 | 0.68                 |                     | 0.66  |
| sulfamate                              | $\text{Ca}(\text{SO}_3\text{NH}_2)_2$                                         | 56.5  | 62.8  | 72.3                 | 84.5                | 100.1               | 150.0                | 215.2                | 242 <sup>95°</sup>  |       |
| sulfate                                | $\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$                           |       |       | 0.32                 | 0.29 <sup>25°</sup> | 0.26 <sup>35°</sup> | 0.21 <sup>45°</sup>  | 0.145 <sup>65°</sup> | 0.12 <sup>75°</sup> | 0.071 |
|                                        | $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$                                     | 0.223 | 0.244 | 0.255 <sup>18°</sup> | 0.264               | 0.265               | 0.244 <sup>65°</sup> | 0.234 <sup>75°</sup> |                     | 0.205 |
| tartrate                               | $\text{CaC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$                  | 0.026 | 0.029 | 0.034                | 0.046               | 0.063               | 0.091                | 0.130                |                     |       |
| uranyl carbonate                       | $\text{Ca}_2\text{UO}_2(\text{CO}_3)_3 \cdot 10\text{H}_2\text{O}$            | 0.1   |       | 0.4 <sup>23</sup>    |                     | 0.8                 | 1.5 <sup>55°</sup>   |                      |                     |       |
| valerate                               | $\text{Ca}(\text{C}_5\text{H}_9\text{O}_2)_2$                                 | 9.82  | 9.25  | 8.80                 | 8.40                | 8.05                | 7.78                 | 7.95                 | 8.20                | 8.78  |
| isovalerate                            | $\text{Ca}(\text{C}_5\text{H}_9\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$       | 26.05 | 22.70 | 21.80                | 21.68               | 22.00               | 18.38                | 16.88                | 16.65               | 16.55 |
| <b>Carbon</b> disulfide                | $\text{CS}_2$                                                                 | 0.204 | 0.194 | 0.179                | 0.155               | 0.111               |                      |                      |                     |       |
| oxide sulfide (STP)<br>mL/100 mL       | $\text{COS}$                                                                  | 133.3 | 83.6  | 56.1                 | 40.3                |                     |                      |                      |                     |       |
| tetrafluoride (STP)<br>mL/100 g        | $\text{CF}_4$                                                                 |       | 0.595 | 0.490                | 0.415               | 0.366               |                      |                      |                     |       |
| <b>Cerium(III)</b> ammonium<br>nitrate | $\text{Ce}(\text{NH}_4)_2(\text{NO}_3)_5$                                     |       | 242   | 276                  | 318                 | 376                 | 681                  |                      |                     |       |
| (IV) ammonium<br>nitrate               | $\text{Ce}(\text{NH}_4)_2(\text{NO}_3)_6$                                     |       |       | 135                  | 150                 | 169                 | 213                  |                      |                     |       |
| (III) ammonium<br>sulfate              | $\text{Ce}(\text{NH}_4)(\text{SO}_4)_2$                                       |       |       | 5.53                 | 4.49                | 3.48                | 2.02                 | 1.33                 |                     |       |
| (III) selenate                         | $\text{Ce}_2(\text{SeO}_3)_3$                                                 | 39.5  | 37.2  | 35.2                 | 33.2                | 32.6                | 13.7                 | 4.6                  | 2.1                 |       |

|                                     |                                                             |                   |                      |                     |                     |                     |        |                     |        |        |
|-------------------------------------|-------------------------------------------------------------|-------------------|----------------------|---------------------|---------------------|---------------------|--------|---------------------|--------|--------|
| (III) sulfate                       | $\text{Ce}_2(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$      | 21.4              |                      | 9.84                | 7.24                | 5.63                | 3.87   |                     |        |        |
|                                     | $\text{Ce}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$      |                   |                      | 9.43                | 7.10                | 5.70                | 4.04   |                     |        |        |
| <b>Cesium</b> aluminum sulfate      | $\text{Cs}_2\text{Al}_2(\text{SO}_4)_4$                     | 18.8              | 0.30                 | 0.40                | 0.61                | 0.85                | 2.00   | 5.40                | 10.5   | 22.7   |
| bromate                             | $\text{CsBrO}_3$                                            | 0.21              |                      | 3.66 <sup>25°</sup> | 4.53                | 5.30 <sup>35°</sup> |        |                     |        |        |
| chlorate                            | $\text{CsClO}_3$                                            |                   | 3.8                  | 6.2                 | 9.5                 | 13.8                | 26.2   | 45.0                | 58.0   | 79.0   |
| chloride                            | $\text{CsCl}$                                               | 2.46              | 175                  | 187                 | 197                 | 208                 | 230    | 250                 | 260    | 271    |
| chloroaurate(III)                   | $\text{CsAuCl}_4$                                           | 161               | 0.5                  | 0.8                 | 1.7                 | 3.3                 | 8.9    | 19.5                | 27.7   | 37.9   |
| chloroplatinate(IV)                 | $\text{Cs}_2\text{PtCl}_6$                                  | 0.0047            | 0.0064               | 0.0087              | 0.0119              | 0.0158              | 0.0290 | 0.0525              | 0.0675 | 0.0914 |
| formate                             | $\text{CsCHO}_2$                                            | 335               | 381                  | 450                 | 533                 | 694                 |        |                     |        |        |
| iodide                              | $\text{CsI}$                                                | 44.1              | 58.5                 | 76.5                | 96                  | 124 <sup>45°</sup>  | 150    | 190                 | 205    |        |
| nitrate                             | $\text{CsNO}_3$                                             | 9.33              | 14.9                 | 23.0                | 33.9                | 47.2                | 83.8   | 134                 | 163    | 197    |
| perchlorate                         | $\text{CsClO}_4$                                            | 0.8               | 1.0                  | 1.6                 | 2.6                 | 4.0                 | 7.3    | 14.4                | 20.5   | 30.0   |
| sulfate                             | $\text{Cs}_2\text{SO}_4$                                    | 167               | 173                  | 179                 | 184                 | 190                 | 200    | 210                 | 215    | 220    |
| <b>Chlorine dioxide</b>             | $\text{ClO}_2$                                              | 2.76              | 6.00                 | 8.70 <sup>15°</sup> |                     |                     |        |                     |        |        |
| <b>Chromium(III)</b> nitrate        | $\text{Cr}(\text{NO}_3)_3$                                  | 108 <sup>5°</sup> | 124 <sup>15°</sup>   | 130 <sup>25°</sup>  | 152 <sup>35°</sup>  |                     |        |                     |        |        |
| (VI) oxide                          | $\text{CrO}_3$                                              | 164.8             |                      | 167.2               |                     | 172.5               | 183.9  | 191.6               |        | 206.8  |
| (III) perchlorate                   | $\text{Cr}(\text{ClO}_4)_3$                                 | 104               | 123                  | 130                 |                     |                     |        |                     |        |        |
| <b>Cobalt(II)</b> bromide           | $\text{CoBr}_2$                                             | 91.9              |                      | 112                 | 128                 | 163                 | 227    | 241                 |        | 257    |
| chlorate                            | $\text{Co}(\text{ClO}_3)_2$                                 | 135               | 162                  | 180                 | 195                 | 214                 | 316    |                     |        |        |
| chloride                            | $\text{CoCl}_2$                                             | 43.5              | 47.7                 | 52.9                | 59.7                | 69.5                | 93.8   | 97.6                | 101    | 106    |
| iodate                              | $\text{Co}(\text{IO}_3)_2$                                  |                   |                      | 1.02                | 0.90                | 0.88                | 0.82   | 0.73                |        | 0.70   |
| nitrate                             | $\text{Co}(\text{NO}_3)_2$                                  | 84.0              | 89.6                 | 97.4                | 111                 | 125                 | 174    | 204                 | 300    |        |
| nitrite                             | $\text{Co}(\text{NO}_2)_2$                                  | 0.076             | 0.24                 | 0.40                | 0.61                | 0.85                |        |                     |        |        |
| sulfate                             | $\text{CoSO}_4$                                             | 25.5              | 30.5                 | 36.1                | 42.0                | 48.8                | 55.0   | 53.8                | 45.3   | 38.9   |
|                                     | $\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$                   | 44.8              | 56.3                 | 65.4                | 73.0                | 88.1                | 101    |                     |        |        |
| <b>Copper(II)</b> ammonium chloride | $\text{CuCl}_2 \cdot 2\text{NH}_4\text{Cl}$                 | 28.2              | 32.0 <sup>12°</sup>  | 35.0                | 38.3                | 43.8                | 56.6   | 76.5                | 76.5   |        |
| ammonium sulfate                    | $\text{CuSO}_4 \cdot (\text{NH}_4)_2\text{SO}_4$            | 11.5              | 15.1                 | 19.4                | 24.4                | 30.5                | 46.3   | 69.7                | 86.1   | 107    |
| bromide                             | $\text{CuBr}_2$                                             | 107               | 116                  | 126                 | 128                 | 131 <sup>50°</sup>  |        |                     |        |        |
| chloride                            | $\text{CuCl}_2$                                             | 68.6              | 70.9                 | 73.0                | 77.3                | 87.6                | 96.5   | 104                 | 108    | 120    |
| fluorosilicate                      | $\text{CuSiF}_6$                                            | 73.5              | 76.5                 | 81.6                | 84.1 <sup>25°</sup> | 91.2 <sup>50°</sup> |        | 93.2 <sup>75°</sup> |        |        |
| nitrate                             | $\text{Cu}(\text{NO}_3)_2$                                  | 83.5              | 100                  | 125                 | 156                 | 163                 | 182    | 208                 | 222    | 247    |
| potassium sulfate                   | $\text{CuSO}_4 \cdot \text{K}_2\text{SO}_4$                 | 5.1               | 7.2                  | 10.0                | 13.6                | 18.2                |        |                     |        |        |
| selenate                            | $\text{CuSeO}_4$                                            | 12.04             | 14.53                | 17.51               | 21.04               | 25.22               | 36.50  | 53.68               |        |        |
| sulfate                             | $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$                   | 23.1              | 27.5                 | 32.0                | 37.8                | 44.6                | 61.8   | 83.8                |        | 114    |
| tartrate                            | $\text{Cu}_2\text{H}_4\text{O}_6 \cdot 3\text{H}_2\text{O}$ |                   | 0.020 <sup>15°</sup> | 0.042               | 0.089               | 0.142               | 0.197  | 0.144               |        |        |
| <b>Gadolinium</b> bromate           | $\text{Gd}(\text{BrO}_3)_3 \cdot 9\text{H}_2\text{O}$       | 50.2              | 70.1                 | 95.6                | 126                 | 166                 |        |                     |        |        |
| sulfate                             | $\text{Gd}_2(\text{SO}_4)_3$                                | 3.98              | 3.30                 | 2.60                | 2.32                |                     |        |                     |        |        |

**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                            | Formula                                                                                 | 0°    | 10°                  | 20°                  | 30°                 | 40°                  | 60°                 | 80°                  | 90°   | 100°                  |
|--------------------------------------|-----------------------------------------------------------------------------------------|-------|----------------------|----------------------|---------------------|----------------------|---------------------|----------------------|-------|-----------------------|
| <b>Germanium(IV) oxide</b>           | GeO <sub>2</sub>                                                                        |       | 0.49                 | 0.43                 | 0.50                | 0.61                 |                     |                      |       |                       |
| <b>Holmium sulfate</b>               | Ho <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O                     |       |                      | 8.18                 | 6.71 <sup>25°</sup> | 4.52                 |                     |                      |       |                       |
| <b>Hydrazinium</b> (1+) nitrate      | N <sub>2</sub> H <sub>5</sub> NO <sub>3</sub>                                           | 175   | 266                  | 402                  | 607                 | 2127                 |                     |                      |       |                       |
| (2+) sulfate                         | N <sub>2</sub> H <sub>6</sub> SO <sub>4</sub>                                           |       | 2.87                 | 3.89                 | 4.15                | 9.08                 | 14.39               |                      |       |                       |
| (1+) sulfate                         | (N <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> SO <sub>4</sub>                           |       |                      | 221                  | 300                 | 554                  |                     |                      |       |                       |
| <b>Hydrogen</b> bromide              | HBr                                                                                     | 221.2 | 210.3                | 204.0 <sup>15°</sup> |                     | 171.5 <sup>50°</sup> |                     | 150.5 <sup>75°</sup> |       | 130.0                 |
| chloride                             | HCl                                                                                     | 82.3  | 77.2                 | 72.1                 | 67.3                | 63.3                 | 56.1                |                      |       |                       |
| selenide, mL at STP                  | H <sub>2</sub> Se                                                                       | 386   | 351                  | 289                  |                     |                      |                     |                      |       |                       |
| <b>Iodine</b>                        | I <sub>2</sub>                                                                          | 0.014 | 0.020                | 0.029                | 0.039               | 0.052                | 0.100               | 0.225                | 0.315 | 0.445                 |
| <b>Iridium(IV)</b> ammonium chloride | (NH <sub>4</sub> ) <sub>2</sub> IrCl <sub>6</sub>                                       | 0.556 | 0.706                | 0.77                 | 1.21                | 1.57                 | 2.46                | 4.38                 | dec   |                       |
| sodium chloride                      | Na <sub>2</sub> IrCl <sub>6</sub>                                                       |       | 34.46 <sup>15°</sup> |                      | 56.17               | 96.00                | 191.2               | 279.3                |       |                       |
| <b>Iron(II)</b> ammonium sulfate     | FeSO <sub>4</sub> · (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> · 6H <sub>2</sub> O | 17.23 | 31.0                 | 36.47                | 45.0                |                      |                     |                      |       |                       |
| (II) bromide                         | FeBr <sub>2</sub>                                                                       | 101   | 109                  | 117                  | 124                 | 133                  | 144                 | 168                  | 176   | 184                   |
| (II) chloride                        | FeCl <sub>2</sub>                                                                       | 49.7  | 59.0                 | 62.5                 | 66.7                | 70.0                 | 78.3                | 88.7                 | 92.3  | 94.9                  |
| (III) chloride                       | FeCl <sub>3</sub> · 6H <sub>2</sub> O                                                   | 74.4  |                      | 91.8                 | 106.8               |                      |                     |                      |       |                       |
| (II) fluoro-silicate                 | FeSiF <sub>6</sub> · 6H <sub>2</sub> O                                                  | 72.1  | 74.4                 |                      | 77.0 <sup>25°</sup> |                      | 83.7 <sup>50°</sup> | 88.1 <sup>75°</sup>  |       | 100.1 <sup>106°</sup> |
| (II) nitrate                         | Fe(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                                   | 113   | 134                  |                      |                     |                      | 266                 |                      |       |                       |
| (III) nitrate                        | Fe(NO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O                                   | 112.0 |                      | 137.7                |                     | 175.0                |                     |                      |       |                       |
| (III) perchlorate                    | Fe(ClO <sub>4</sub> ) <sub>3</sub>                                                      | 289   |                      | 368                  | 422                 | 478                  | 772                 |                      |       |                       |
| (II) sulfate                         | FeSO <sub>4</sub> · 7H <sub>2</sub> O                                                   | 28.8  | 40.0                 | 48.0                 | 60.0                | 73.3                 | 100.7               | 79.9                 | 68.3  | 57.8                  |
| <b>Lanthanum</b> bromate             | La(BrO <sub>3</sub> ) <sub>3</sub>                                                      | 98    | 120                  | 149                  | 200                 |                      |                     |                      |       |                       |
| nitrate                              | La(NO <sub>3</sub> ) <sub>3</sub>                                                       | 100   |                      | 136                  |                     | 168                  | 247                 |                      |       |                       |
| selenate                             | La <sub>2</sub> (SeO <sub>3</sub> ) <sub>3</sub>                                        | 50.5  | 45                   | 45                   | 45                  | 45                   | 18.5                | 5.4                  | 2.2   |                       |
| sulfate                              | La <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                                         | 3.00  | 2.72                 | 2.33                 | 1.90                | 1.67                 | 1.26                | 0.91                 | 0.79  | 0.68                  |
| <b>Lead(II)</b> acetate              | Pb(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub>                          | 19.8  | 29.5                 | 44.3                 | 69.8                | 116                  |                     |                      |       |                       |
| bromide                              | PbBr <sub>2</sub>                                                                       | 0.45  | 0.63                 | 0.86                 | 1.12                | 1.50                 | 2.29                | 3.23                 | 3.86  | 4.55                  |
| chloride                             | PbCl <sub>2</sub>                                                                       | 0.67  | 0.82                 | 1.00                 | 1.20                | 1.42                 | 1.94                | 2.54                 | 2.88  | 3.20                  |
| fluorosilicate                       | PbSiF <sub>6</sub>                                                                      | 190   |                      | 222                  |                     |                      | 403                 | 428                  |       | 463                   |

|                          |                                                                |       |       |                      |       |       |       |       |      |       |
|--------------------------|----------------------------------------------------------------|-------|-------|----------------------|-------|-------|-------|-------|------|-------|
| iodide                   | PbI <sub>2</sub>                                               | 0.044 | 0.056 | 0.069                | 0.090 | 0.124 | 0.193 | 0.294 |      | 0.42  |
| nitrate                  | Pb(NO <sub>3</sub> ) <sub>2</sub>                              | 37.5  | 46.2  | 54.3                 | 63.4  | 72.1  | 91.6  | 111   |      | 133   |
| <b>Lithium</b> acetate   | LiC <sub>2</sub> H <sub>3</sub> O <sub>2</sub>                 | 31.2  | 35.1  | 40.8                 | 50.6  | 68.6  |       |       |      |       |
| ammonium sulfate         | LiNH <sub>4</sub> SO <sub>4</sub>                              |       | 55.2  |                      | 55.9  | 56.1  | 56.5  |       |      |       |
| azide                    | LiN <sub>3</sub>                                               | 61.3  | 64.2  | 67.2                 | 71.2  | 75.4  | 86.6  |       |      | 100   |
| benzoate                 | LiC <sub>7</sub> H <sub>5</sub> O <sub>2</sub>                 | 38.9  | 41.6  | 44.7                 | 53.8  |       |       |       |      |       |
| borate (meta-)           | LiBO <sub>2</sub>                                              | 0.90  | 1.3   | 2.7                  | 5.7   | 10.9  |       |       |      |       |
| bromate                  | LiBrO <sub>3</sub>                                             | 154   | 166   | 179                  | 198   | 221   | 269   | 308   | 329  | 355   |
| bromide                  | LiBr                                                           | 143   | 147   | 160                  | 183   | 211   | 223   | 245   |      | 266   |
| carbonate                | Li <sub>2</sub> CO <sub>3</sub>                                | 1.54  | 1.43  | 1.33                 | 1.26  | 1.17  | 1.01  | 0.85  |      | 0.72  |
| chlorate                 | LiClO <sub>3</sub>                                             | 241   | 283   | 372                  | 488   | 604   | 777   |       |      |       |
| chloride                 | LiCl                                                           | 69.2  | 74.5  | 83.5                 | 86.2  | 89.8  | 98.4  | 112   | 121  | 128   |
| chloroaurate(III)        | LiAuCl <sub>4</sub>                                            |       | 113   | 136                  | 167   | 206   | 324   | 599   |      |       |
| cyanoplatinate(II)       | Li <sub>2</sub> Pt(CN) <sub>4</sub>                            | 105   |       | 141                  | 153   | 160   | 178   | 216   | 239  |       |
| formate                  | LiCHO <sub>2</sub>                                             | 32.3  | 35.7  | 39.3                 | 44.1  | 49.5  | 64.7  | 92.7  | 116  | 138   |
| hydrogen phosphite       | Li <sub>2</sub> HPO <sub>3</sub>                               | 9.97  |       |                      | 7.61  | 7.11  | 6.03  |       |      | 4.43  |
| hydroxide                | LiOH                                                           | 11.91 | 12.11 | 12.35                | 12.70 | 13.22 | 14.63 | 16.56 |      | 19.12 |
| iodide                   | LiI                                                            | 151   | 157   | 165                  | 171   | 179   | 202   | 435   | 440  | 481   |
| molybdate                | Li <sub>2</sub> MoO <sub>4</sub>                               | 82.6  |       | 79.5                 | 79.4  | 78.0  |       |       |      | 73.9  |
| nitrate                  | LiNO <sub>3</sub>                                              | 53.4  | 60.8  | 70.1                 | 138   | 152   | 175   |       |      |       |
| nitrite                  | LiNO <sub>2</sub>                                              | 70.9  | 82.5  | 96.8                 | 114   | 133   | 177   | 233   | 272  | 324   |
| perchlorate              | LiClO <sub>4</sub>                                             | 42.7  | 49.0  | 56.1                 | 63.6  | 72.3  | 92.3  | 128   | 151  |       |
| phosphate (meta-)        | LiPO <sub>3</sub>                                              | 0.101 |       | 0.058 <sup>25°</sup> |       | 0.048 |       |       |      |       |
| selenite                 | Li <sub>2</sub> SeO <sub>3</sub>                               | 25.0  | 23.3  | 21.5                 | 19.6  | 17.9  | 14.7  | 11.9  | 11.1 | 9.9   |
| sulfate                  | Li <sub>2</sub> SO <sub>4</sub>                                | 36.1  | 35.5  | 34.8                 | 34.2  | 33.7  | 32.6  | 31.4  | 30.9 |       |
| tartrate ( <i>d</i> -)   | Li <sub>2</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub>   | 42.0  | 31.8  | 27.1                 | 26.6  | 27.2  | 29.5  |       |      |       |
| thiocyanate              | LiSCN                                                          |       |       | 114                  | 131   | 153   |       |       |      |       |
| vanadate                 | Li <sub>3</sub> VO <sub>4</sub>                                | 2.50  |       | 4.82                 | 6.28  | 4.38  | 2.67  |       |      |       |
| <b>Magnesium</b> acetate | Mg(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> | 56.7  | 59.7  | 53.4                 | 68.6  | 75.7  | 118   |       |      |       |
| bromide                  | MgBr <sub>2</sub>                                              | 98    | 99    | 101                  | 104   | 106   | 112   |       |      | 125   |
| chlorate                 | Mg(ClO <sub>3</sub> ) <sub>2</sub>                             | 114   | 123   | 135                  | 155   | 178   | 242   |       | 268  |       |
| chloride                 | MgCl <sub>2</sub>                                              | 52.9  | 53.6  | 54.6                 | 55.8  | 57.5  | 61.0  | 66.1  | 69.5 | 73.3  |
| fluorosilicate           | MgSiF <sub>6</sub>                                             | 26.3  |       | 30.8                 |       | 34.9  | 44.4  |       |      |       |
| formate                  | Mg(CHO <sub>2</sub> ) <sub>2</sub>                             | 14.0  | 14.2  | 14.4                 | 14.9  | 15.9  | 17.9  | 20.5  | 22.2 | 23.9  |
| iodate                   | Mg(IO <sub>3</sub> ) <sub>2</sub>                              |       | 7.2   | 8.6                  | 10.0  | 11.7  | 15.2  | 15.5  | 15.6 |       |
| iodide                   | MgI <sub>2</sub>                                               | 120   |       | 140                  |       | 173   |       | 186   |      |       |

**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                  | Formula                                               | 0°    | 10°   | 20°   | 30°   | 40°   | 60°   | 80°   | 90°   | 100° |
|----------------------------|-------------------------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|------|
| <b>Magnesium</b> nitrate   | Mg(NO <sub>3</sub> ) <sub>2</sub>                     | 62.1  | 66.0  | 69.5  | 73.6  | 78.9  | 78.9  | 91.6  | 106   |      |
| selenate                   | MgSeO <sub>4</sub>                                    | 20.0  | 30.4  | 38.3  | 44.3  | 48.6  | 55.8  |       |       |      |
| sulfate                    | MgSO <sub>4</sub>                                     | 22.0  | 28.2  | 33.7  | 38.9  | 44.5  | 54.6  | 55.8  | 52.9  | 50.4 |
| sulfite                    | MgSO <sub>3</sub>                                     | 0.339 | 0.446 | 0.573 | 0.751 | 0.959 | 0.779 | 0.642 | 0.622 |      |
| tartrate                   | MgC <sub>4</sub> H <sub>4</sub> O <sub>6</sub>        | 0.54  | 0.78  | 1.06  |       | 1.02  |       |       |       |      |
| <b>Manganese</b> bromide   | MnBr <sub>2</sub>                                     | 127   | 136   | 147   | 157   | 169   | 197   | 225   | 226   | 228  |
| chloride                   | MnCl <sub>2</sub>                                     | 63.4  | 68.1  | 73.9  | 80.8  | 88.5  | 109   | 113   | 114   | 115  |
| fluoride                   | MnF <sub>2</sub>                                      |       |       | 1.06  |       | 0.67  | 0.44  |       |       | 0.48 |
| nitrate                    | Mn(NO <sub>3</sub> ) <sub>2</sub>                     | 102   | 118   | 139   | 206   |       |       |       |       |      |
| oxalate                    | MnC <sub>2</sub> O <sub>4</sub>                       | 0.020 | 0.024 | 0.028 | 0.033 |       |       |       |       |      |
| sulfate                    | MnSO <sub>4</sub>                                     | 52.9  | 59.7  | 62.9  | 62.9  | 60.0  | 53.6  | 45.6  | 40.9  | 35.3 |
| <b>Mercury(II)</b> bromide | HgBr <sub>2</sub>                                     | 0.30  | 0.40  | 0.56  | 0.66  | 0.91  | 1.68  | 2.77  |       | 4.9  |
| (II) chloride              | HgCl <sub>2</sub>                                     | 3.63  | 4.82  | 6.57  | 8.34  | 10.2  | 16.3  | 30.0  |       | 61.3 |
| (I) perchlorate            | Hg <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub>      | 282   | 325   | 367   | 407   | 455   | 499   | 541   |       | 580  |
| <b>Molybdenum trioxide</b> | MoO <sub>3</sub>                                      |       |       | 0.134 | 0.285 | 0.454 | 1.08  | 1.74  |       |      |
| <b>Neodymium</b> bromate   | Nd(BrO <sub>3</sub> ) <sub>3</sub>                    | 43.9  | 59.2  | 75.6  | 95.2  | 116   |       |       |       |      |
| chloride                   | NdCl <sub>3</sub>                                     |       | 96.7  | 98.0  | 99.6  | 102   | 105   |       |       |      |
| nitrate                    | Nd(NO <sub>3</sub> ) <sub>3</sub>                     | 127   | 133   | 142   | 145   | 159   | 211   |       |       |      |
| selenate                   | Nd <sub>2</sub> (SeO <sub>3</sub> ) <sub>3</sub>      | 46.2  | 44.6  | 41.8  | 39.9  | 39.9  | 43.9  | 7.0   | 3.3   |      |
| sulfate                    | Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>       | 13.0  | 9.7   | 7.1   | 5.3   | 4.1   | 2.8   | 2.2   | 1.2   |      |
| <b>Nickel</b> bromide      | NiBr <sub>2</sub>                                     | 113   | 122   | 131   | 138   | 144   | 153   | 154   |       | 155  |
| chlorate                   | Ni(ClO <sub>3</sub> ) <sub>2</sub>                    | 111   | 120   | 133   | 155   | 181   | 221   | 308   |       |      |
| chloride                   | NiCl <sub>2</sub>                                     | 53.4  | 56.3  | 60.8  | 70.6  | 73.2  | 81.2  | 86.6  |       | 87.6 |
| fluoride                   | NiF <sub>2</sub>                                      |       | 2.55  | 2.56  |       |       | 2.56  |       | 2.59  |      |
| iodate                     | Ni(IO <sub>3</sub> ) <sub>2</sub>                     |       |       |       | 1.15  |       | 1.06  |       | 1.00  |      |
|                            | Ni(IO <sub>3</sub> ) <sub>2</sub> · 4H <sub>2</sub> O | 0.74  |       | 1.09  | 1.43  |       |       |       |       |      |
| iodide                     | NiI <sub>2</sub>                                      | 124   | 135   | 148   | 161   | 174   | 184   | 187   | 188   |      |
| nitrate                    | Ni(NO <sub>3</sub> ) <sub>2</sub>                     | 79.2  |       | 94.2  | 105   | 119   | 158   | 187   | 188   |      |
| perchlorate                | Ni(ClO <sub>4</sub> ) <sub>2</sub>                    | 105   | 107   | 110   | 113   | 117   |       |       |       |      |

|                          |                                                             |             |       |       |       |       |       |      |      |      |  |
|--------------------------|-------------------------------------------------------------|-------------|-------|-------|-------|-------|-------|------|------|------|--|
| <b>Nickel</b> sulfate    | NiSO <sub>4</sub> · 6H <sub>2</sub> O                       | (pale blue) |       | 40.1  | 43.6  | 47.6  |       |      |      |      |  |
|                          |                                                             | (green)     |       | 44.4  | 46.6  | 49.2  | 55.6  | 64.5 | 70.1 | 76.7 |  |
|                          | NiSO <sub>4</sub> · 7H <sub>2</sub> O                       | 26.2        | 32.4  | 37.7  | 43.4  | 50.4  |       |      |      |      |  |
| <b>Osmium tetroxide</b>  | OsO <sub>4</sub>                                            | 5.26        | 5.75  | 6.43  |       |       |       |      |      |      |  |
| <b>Oxalic acid</b>       | H <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                | 3.54        | 6.08  | 9.52  | 14.23 | 21.52 | 44.32 | 84.5 | 120  |      |  |
| <b>Potassium</b> acetate | KC <sub>2</sub> H <sub>3</sub> O <sub>2</sub>               | 216         | 233   | 256   | 283   | 324   | 350   | 381  | 398  |      |  |
| aluminum sulfate         | KAl(SO <sub>4</sub> ) <sub>2</sub>                          | 3.00        | 3.99  | 5.90  | 8.39  | 11.7  | 24.8  | 71.0 | 109  |      |  |
| azide                    | KN <sub>3</sub>                                             | 41.4        | 46.2  | 50.8  | 55.8  | 61.0  |       |      |      | 106  |  |
| benzoate                 | KC <sub>7</sub> H <sub>5</sub> O <sub>2</sub>               |             | 65.8  | 70.7  | 76.7  | 82.1  |       |      |      |      |  |
| bromate                  | KBrO <sub>3</sub>                                           | 3.09        | 4.72  | 6.91  | 9.64  | 13.1  | 22.7  | 34.1 |      | 49.9 |  |
| bromide                  | KBr                                                         | 53.6        | 59.5  | 65.3  | 70.7  | 75.4  | 85.5  | 94.9 | 99.2 | 104  |  |
| cadmium bromide          | KCdBr <sub>3</sub>                                          | 116         | 133   | 150   | 170   | 191   | 233   | 276  | 298  | 325  |  |
| cadmium chloride         | KCdCl <sub>3</sub>                                          | 26.6        | 32.3  | 38.9  | 45.6  | 53.1  | 67.5  | 83.5 |      | 101  |  |
| carbonate                | K <sub>2</sub> CO <sub>3</sub>                              | 105         | 108   | 111   | 114   | 117   | 127   | 140  | 148  | 156  |  |
| chlorate                 | KClO <sub>3</sub>                                           | 3.3         | 5.2   | 7.3   | 10.1  | 13.9  | 23.8  | 37.6 | 46.0 | 56.3 |  |
| chloride                 | KCl                                                         | 28.0        | 31.2  | 34.2  | 37.2  | 40.1  | 45.8  | 51.3 | 53.9 | 56.3 |  |
| chloroaurate(III)        | KAuCl <sub>4</sub>                                          |             | 38.3  | 61.8  | 94.9  | 145   | 405   |      |      |      |  |
| chloroplatinate(IV)      | K <sub>2</sub> PtCl <sub>6</sub>                            | 0.48        | 0.60  | 0.78  | 1.00  | 1.36  | 2.45  | 3.71 |      | 5.03 |  |
| chromate                 | K <sub>2</sub> CrO <sub>4</sub>                             | 56.3        | 60.0  | 63.7  | 66.7  | 67.8  | 70.1  |      | 74.5 |      |  |
| citrate                  | K <sub>3</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> |             | 153   | 172   | 194   |       |       |      |      |      |  |
| cobalt(II) sulfate       | K <sub>2</sub> Co(SO <sub>4</sub> ) <sub>2</sub>            | 8.5         | 11.7  | 15.5  | 19.3  | 23.3  | 32.5  | 47.7 |      |      |  |
| copper(II) sulfate       | K <sub>2</sub> Cu(SO <sub>4</sub> ) <sub>2</sub>            | 5.1         | 7.2   | 10.0  | 13.6  | 18.2  |       |      |      |      |  |
| cyanoplatinate(II)       | K <sub>2</sub> Pt(CN) <sub>4</sub>                          | 11.6        | 19.8  | 33.9  | 52.0  | 78.3  | 139   | 177  | 194  |      |  |
| dichromate               | K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>               | 4.7         | 7.0   | 12.3  | 18.1  | 26.3  | 45.6  | 73.0 |      |      |  |
| dihydrogen phosphate     | KH <sub>2</sub> PO <sub>4</sub>                             | 14.8        | 18.3  | 22.6  | 28.0  | 33.5  | 50.2  | 70.4 | 83.5 |      |  |
| dithionate               | K <sub>2</sub> S <sub>2</sub> O <sub>6</sub>                | 2.6         | 4.2   | 6.6   | 9.3   |       |       |      |      |      |  |
| ferricyanide             | K <sub>3</sub> Fe(CN) <sub>6</sub>                          | 30.2        | 38    | 46    | 53    | 59.3  | 70    |      |      | 91   |  |
| ferrocyanide             | K <sub>4</sub> Fe(CN) <sub>6</sub>                          | 14.3        | 21.1  | 28.2  | 35.1  | 41.4  | 54.8  | 66.9 | 71.5 | 74.2 |  |
| fluoride                 | KF                                                          | 44.7        | 53.5  | 94.9  | 108   | 138   | 142   | 150  |      |      |  |
| fluorogermanate(IV)      | K <sub>2</sub> GeF <sub>6</sub>                             | 0.25        | 0.36  | 0.50  | 0.66  | 0.96  |       |      |      |      |  |
| fluorosilicate           | K <sub>2</sub> SiF <sub>6</sub>                             | 0.077       | 0.102 | 0.151 | 0.202 | 0.253 |       |      |      |      |  |
| fluorotitanate(IV)       | K <sub>2</sub> TiF <sub>6</sub>                             | 0.55        | 0.91  | 1.28  |       |       |       |      |      |      |  |
| formate                  | KCHO <sub>2</sub>                                           |             | 313   | 337   | 361   | 398   | 471   | 580  | 658  |      |  |
| hydrogen carbonate       | KHCO <sub>3</sub>                                           | 22.5        | 27.4  | 33.7  | 39.9  | 47.5  | 65.6  |      |      |      |  |

**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                          | Formula                                                              | 0°    | 10°   | 20°   | 30°   | 40°  | 60°  | 80°  | 90°  | 100° |
|------------------------------------|----------------------------------------------------------------------|-------|-------|-------|-------|------|------|------|------|------|
| <b>Potassium</b> hydrogen fluoride | KHF <sub>2</sub>                                                     | 24.5  | 30.1  | 39.2  | 46.8  | 56.5 | 78.8 | 114  |      |      |
| hydrogen selenite                  | KH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>                     | 115   | 162   | 215   | 300   | 408  | 900  |      |      |      |
| hydrogen sulfate                   | KHSO <sub>4</sub>                                                    | 36.2  |       | 48.6  | 54.3  | 61.0 | 76.4 | 96.1 |      | 122  |
| hydrogen tartrate                  | KC <sub>4</sub> H <sub>3</sub> O <sub>6</sub>                        | 0.231 | 0.358 | 0.523 | 0.762 |      |      |      |      |      |
| hydroxide                          | KOH                                                                  | 95.7  | 103   | 112   | 126   | 134  | 154  |      |      | 178  |
| iodate                             | KIO <sub>3</sub>                                                     | 4.60  | 6.27  | 8.08  | 10.3  | 12.6 | 18.3 | 24.8 |      | 32.3 |
| iodide                             | KI                                                                   | 128   | 136   | 144   | 153   | 162  | 176  | 192  | 198  | 206  |
| iron(II) sulfate                   | K <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub>                     | 19.6  | 24.5  | 32.1  | 39.1  | 44.9 | 57.2 |      |      |      |
| magnesium sulfate                  | K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub>                     | 14.0  | 19.5  | 25.0  | 30.4  | 36.6 | 50.2 | 63.4 |      |      |
| nickel sulfate                     | K <sub>2</sub> Ni(SO <sub>4</sub> ) <sub>2</sub>                     | 3.37  | 4.50  | 5.94  | 7.72  | 9.85 | 15.4 | 23.0 | 27.8 | 33.4 |
| nitrate                            | KNO <sub>3</sub>                                                     | 13.9  | 21.2  | 31.6  | 45.3  | 61.3 | 106  | 167  | 203  | 245  |
| nitrite                            | KNO <sub>2</sub>                                                     | 279   | 292   | 306   | 320   | 329  | 348  | 376  | 390  | 410  |
| oxalate                            | K <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                         | 25.5  | 31.9  | 36.4  | 39.9  | 43.8 | 53.2 | 63.6 | 69.2 | 75.3 |
| perchlorate                        | KClO <sub>4</sub>                                                    | 0.76  | 1.06  | 1.68  | 2.56  | 3.73 | 7.3  | 13.4 | 17.7 | 22.3 |
| periodate                          | KIO <sub>4</sub>                                                     | 0.17  | 0.28  | 0.42  | 0.65  | 1.0  | 2.1  | 4.4  | 5.9  |      |
| permanganate                       | KMnO <sub>4</sub>                                                    | 2.83  | 4.31  | 6.34  | 9.03  | 12.6 | 22.1 |      |      |      |
| peroxodisulfate                    | K <sub>2</sub> S <sub>2</sub> O <sub>8</sub>                         | 1.65  | 2.67  | 4.70  | 7.75  | 11.0 |      |      |      |      |
| perrhenate                         | KReO <sub>4</sub>                                                    | 0.34  | 0.63  | 0.99  | 1.47  | 2.2  | 4.58 | 8.7  |      |      |
| phosphate                          | K <sub>3</sub> PO <sub>4</sub>                                       |       | 81.5  | 92.3  | 108   | 133  |      |      |      |      |
| salicylate                         | KC <sub>7</sub> H <sub>3</sub> O <sub>3</sub>                        | 21.2  | 32.4  | 47.1  | 61.3  | 78.6 | 116  | 156  |      |      |
| selenate                           | K <sub>2</sub> SeO <sub>4</sub>                                      | 107   | 109   | 111   | 113   | 115  | 119  | 121  |      | 122  |
| selenite                           | K <sub>2</sub> SeO <sub>3</sub>                                      | 169   | 186   | 203   | 217   | 217  | 220  |      |      | 217  |
| sulfate                            | K <sub>2</sub> SO <sub>4</sub>                                       | 7.4   | 9.3   | 11.1  | 13.0  | 14.8 | 18.2 | 21.4 | 22.9 | 24.1 |
| sulfite                            | K <sub>2</sub> SO <sub>3</sub>                                       | 106   |       | 106   | 107   | 107  | 108  |      |      | 112  |
| tellurate                          | K <sub>2</sub> TeO <sub>4</sub>                                      | 8.8   |       | 27.5  | 50.4  |      |      |      |      |      |
| thioantimonate(V)                  | K <sub>3</sub> SbS <sub>4</sub>                                      | 306   | 320   |       | 302   | 315  |      | 381  |      |      |
| thiocyanate                        | KSCN                                                                 | 177   | 198   | 224   | 255   | 289  | 372  | 492  | 571  | 675  |
| thiosulfate                        | K <sub>2</sub> S <sub>2</sub> O <sub>3</sub>                         | 96    |       | 155   | 175   | 205  | 238  | 293  | 312  |      |
| zinc sulfate                       | K <sub>2</sub> Zn(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O | 13.0  | 18.9  | 25.9  | 35.0  | 44.9 | 72.1 |      |      |      |

|                             |                                                                 |       |       |       |       |       |       |       |       |       |
|-----------------------------|-----------------------------------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| <b>Praseodymium</b> bromate | Pr(BrO <sub>3</sub> ) <sub>3</sub>                              | 55.9  | 73.0  | 91.8  | 114   | 144   |       |       |       |       |
| nitrate                     | Pr(NO <sub>3</sub> ) <sub>3</sub>                               |       |       | 112   | 162   | 178   |       |       |       |       |
| selenate                    | Pr <sub>2</sub> (SeO <sub>3</sub> ) <sub>3</sub>                | 36.2  |       |       | 32.4  | 31.2  | 30.4  | 5.43  | 3.6   |       |
| sulfate                     | Pr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                 | 19.8  | 15.6  | 12.6  | 9.89  | 2.56  | 5.04  | 3.5   | 1.1   | 0.91  |
| <b>Rubidium</b> aluminum    |                                                                 |       |       |       |       |       |       |       |       |       |
| sulfate                     | Rb <sub>2</sub> Al <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub> | 0.72  | 1.05  | 1.50  | 2.20  | 3.25  | 7.40  | 21.6  |       |       |
| bromate                     | RbBrO <sub>3</sub>                                              |       |       |       | 3.6   | 5.1   |       |       |       |       |
| bromide                     | RbBr                                                            | 90    | 99    | 108   | 119   | 132   | 158   |       |       |       |
| chlorate                    | RbClO <sub>3</sub>                                              | 2.1   | 3.4   | 5.4   | 8.0   | 11.6  | 22    | 38    | 49    | 63    |
| chloride                    | RbCl                                                            | 77    | 84    | 91    | 98    | 104   | 115   | 127   | 133   | 143   |
| chloroaurate(III)           | RbAuCl <sub>4</sub>                                             |       | 4.8   | 9.9   | 15.5  | 21.5  | 36.2  | 54.6  | 65.8  | 79.2  |
| chloroplatinate(IV)         | Rb <sub>2</sub> PtCl <sub>6</sub>                               | 0.014 | 0.020 | 0.028 | 0.040 | 0.056 | 0.090 | 0.182 | 0.247 | 0.333 |
| chromate                    | Rb <sub>2</sub> CrO <sub>4</sub>                                | 62.0  | 67.5  | 73.6  | 78.9  | 85.6  | 95.7  |       |       |       |
| cobalt sulfate              | Rb <sub>2</sub> Co(SO <sub>4</sub> ) <sub>2</sub>               | 5.10  | 7.47  | 10.8  | 14.5  | 18.2  | 30.2  | 44.9  | 55.0  | 70.1  |
| dichromate (mn)             | Rb <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>                  |       |       | 5.9   | 10.0  | 15.2  | 32.3  |       |       |       |
| (tric)                      |                                                                 |       |       | 5.8   | 9.5   | 14.8  | 32.4  |       |       |       |
| formate                     | RbCHO <sub>2</sub>                                              |       | 443   | 554   | 614   | 694   | 900   |       |       |       |
| iron(III) sulfate           | RbFe(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O        |       | 8.0   | 20    | 35    | 52    |       |       |       |       |
| nitrate                     | RbNO <sub>3</sub>                                               | 19.5  | 33.0  | 52.9  | 81.2  | 117   | 200   | 310   | 374   | 452   |
| perchlorate                 | RbClO <sub>4</sub>                                              | 1.09  | 1.19  | 1.55  | 2.20  | 3.26  | 6.27  | 11.0  | 15.5  | 22.0  |
| salicylate                  | RbC <sub>7</sub> H <sub>5</sub> O <sub>3</sub>                  |       | 187   | 212   | 238   | 268   | 324   |       |       |       |
| sulfate                     | Rb <sub>2</sub> SO <sub>4</sub>                                 | 37.5  | 42.6  | 48.1  | 53.6  | 58.5  | 67.5  | 75.1  | 78.6  | 81.8  |
| <b>Samarium</b> bromate     | Sm(BrO <sub>3</sub> ) <sub>3</sub>                              | 34.2  | 47.6  | 62.5  | 79.0  | 98.5  |       |       |       |       |
| chloride                    | SmCl <sub>3</sub>                                               |       | 92.4  | 93.4  | 94.6  | 96.9  |       |       |       |       |
| <b>Selenic acid</b>         | H <sub>2</sub> SeO <sub>4</sub>                                 | 426   |       | 567   | 1328  |       |       |       |       |       |
| <b>Selenious acid</b>       | H <sub>2</sub> SeO <sub>3</sub>                                 | 90.1  | 122.2 | 166.7 | 235.6 | 344.4 | 383.1 | 383.1 | 385.4 |       |
| <b>Selenium dioxide</b>     | SeO <sub>2</sub>                                                |       | 222   | 257   | 291   | 335   | 440   |       |       |       |
| <b>Silver</b> acetate       | AgC <sub>2</sub> H <sub>3</sub> O <sub>2</sub>                  | 0.73  | 0.89  | 1.05  | 1.23  | 1.43  | 1.93  | 2.59  |       |       |
| bromate                     | AgBrO <sub>3</sub>                                              |       | 0.11  | 0.16  | 0.23  | 0.32  | 0.57  | 0.94  | 1.33  |       |
| chlorate                    | AgClO <sub>3</sub>                                              |       | 10.4  | 15.3  | 20.9  | 26.8  |       |       |       |       |
| fluoride                    | AgF                                                             | 85.9  | 120   | 172   | 190   | 203   |       |       |       |       |
| nitrate                     | AgNO <sub>3</sub>                                               | 122   | 167   | 216   | 265   | 311   | 440   | 585   | 652   | 733   |
| nitrite                     | AgNO <sub>2</sub>                                               | 0.16  | 0.22  | 0.34  | 0.51  | 0.73  | 1.39  |       |       |       |
| perchlorate                 | AgClO <sub>4</sub>                                              | 455   | 484   | 525   | 594   | 635   |       |       |       | 793   |
| sulfamate                   | AgNH <sub>2</sub> SO <sub>3</sub>                               | 2.30  | 4.82  | 7.53  | 10.3  | 15.3  | 28.5  |       |       |       |
| sulfate                     | Ag <sub>2</sub> SO <sub>4</sub>                                 | 0.57  | 0.70  | 0.80  | 0.89  | 0.98  | 1.15  | 1.30  | 1.36  | 1.41  |



**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                        | Formula                                                         | 0°   | 10°  | 20°  | 30°  | 40°  | 60°  | 80°  | 90°  | 100°                |
|----------------------------------|-----------------------------------------------------------------|------|------|------|------|------|------|------|------|---------------------|
| <b>Sodium</b> acetate            | NaC <sub>2</sub> H <sub>3</sub> O <sub>2</sub>                  | 36.2 | 40.8 | 46.4 | 54.6 | 65.6 | 139  | 153  | 161  | 170                 |
| aluminum sulfate                 | Na <sub>2</sub> Al <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub> | 37.4 | 39.3 | 39.7 | 41.7 | 43.8 |      |      |      |                     |
| azide                            | NaN <sub>3</sub>                                                | 38.9 | 39.9 | 40.8 |      |      |      |      |      | 55.3                |
| benzoate                         | NaC <sub>7</sub> H <sub>5</sub> O <sub>2</sub>                  | 62.6 | 62.8 | 62.8 | 62.9 | 63.1 | 64.5 | 68.6 | 70.6 | 73.3                |
| borate (penta-)                  | Na <sub>2</sub> B <sub>10</sub> O <sub>16</sub>                 | 6.4  | 8.6  | 12.0 | 16.4 | 22.0 | 37.9 | 63.4 | 83.5 | 108                 |
| borate (tetra-)                  | Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                   | 1.11 | 1.60 | 2.56 | 3.86 | 6.67 | 19.0 | 31.4 | 41.0 | 52.5                |
| bromate                          | NaBrO <sub>3</sub>                                              | 24.2 | 30.3 | 36.4 | 42.6 | 48.8 | 62.6 | 75.7 |      | 90.8                |
| bromide                          | NaBr                                                            | 80.2 | 85.2 | 90.8 | 98.4 | 107  | 118  | 120  | 121  | 121                 |
| carbonate                        | Na <sub>2</sub> CO <sub>3</sub>                                 | 7.00 | 12.5 | 21.5 | 39.7 | 49.0 | 46.0 | 43.9 | 43.9 |                     |
| chlorate                         | NaClO <sub>3</sub>                                              | 79.6 | 87.6 | 95.9 | 105  | 115  | 137  | 167  | 184  | 204                 |
| chloride                         | NaCl                                                            | 35.7 | 35.8 | 35.9 | 36.1 | 36.4 | 37.1 | 38.0 | 38.5 | 39.2                |
| chloroaurate(III)                | NaAuCl <sub>4</sub>                                             |      | 139  | 151  | 178  | 227  | 900  |      |      |                     |
| chloroiridate(IV)                | Na <sub>2</sub> IrCl <sub>6</sub>                               |      | 31.6 | 39.3 | 56.2 | 96.1 | 192  | 279  |      |                     |
| chromate                         | Na <sub>2</sub> CrO <sub>4</sub>                                | 31.7 | 50.1 | 84.0 | 88.0 | 96.0 | 115  | 125  |      | 126                 |
| cyanide                          | NaCN                                                            | 40.8 | 48.1 | 58.7 | 71.2 |      |      |      |      |                     |
| dichromate                       | Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>                  | 163  | 172  | 183  | 198  | 215  | 269  | 376  | 405  | 415                 |
| diethyl barbiturate              | NaC <sub>8</sub> H <sub>11</sub> N <sub>2</sub> O <sub>3</sub>  |      | 12.7 | 21.5 | 24.7 |      |      |      | 48.0 |                     |
| dihydrogen<br>phosphate (ortho-) | NaH <sub>2</sub> PO <sub>4</sub>                                | 56.5 | 69.8 | 86.9 | 107  | 133  | 172  | 211  | 234  |                     |
| dihydrogen<br>phosphate (pyro-)  | Na <sub>2</sub> H <sub>2</sub> P <sub>2</sub> O <sub>7</sub>    | 4.47 | 6.95 | 12.0 | 17.1 | 18.4 |      |      |      |                     |
| dithionate                       | Na <sub>2</sub> S <sub>2</sub> O <sub>6</sub>                   | 6.3  | 11.1 | 15.1 | 19.6 | 24.7 | 36.1 | 49.3 | 56.3 | 64.7                |
| dodecanesulfonate                | NaC <sub>12</sub> H <sub>25</sub> SO <sub>3</sub>               |      |      | 0.13 | 0.25 | 6.54 |      |      |      |                     |
| dodecanoate                      | NaC <sub>12</sub> H <sub>23</sub> O <sub>2</sub>                |      |      |      | 4.58 | 22.7 | 105  | 170  |      |                     |
| EDTA (Y)*                        | Na <sub>2</sub> H <sub>2</sub> Y · 2H <sub>2</sub> O            | 10.6 |      | 11.1 | 12.8 | 14.2 | 17.0 | 22.2 | 24.3 | 27.0 <sup>98°</sup> |
| ferrocyanide                     | Na <sub>4</sub> Fe(CN) <sub>6</sub>                             | 11.2 | 14.8 | 18.8 | 23.8 | 29.9 | 43.7 | 62.1 |      |                     |
| fluoride                         | NaF                                                             | 3.66 |      | 4.06 | 4.22 | 4.40 | 4.68 | 4.89 |      | 5.08                |
| fluoroberyllate                  | Na <sub>2</sub> BeF <sub>4</sub>                                | 1.33 |      | 1.44 |      | 1.92 | 2.24 | 2.62 | 2.73 |                     |
| fluorogermanate                  | Na <sub>2</sub> GeF <sub>6</sub>                                | 1.52 | 1.68 |      | 2.25 | 2.83 |      | 3.36 |      |                     |
| fluorosilicate                   | Na <sub>2</sub> SiF <sub>6</sub>                                | 4.35 | 5.7  | 7.2  | 8.6  | 10.3 | 14.3 | 18.7 | 21.5 | 24.5                |

|                          |                                                                   |      |       |       |      |      |      |       |      |      |
|--------------------------|-------------------------------------------------------------------|------|-------|-------|------|------|------|-------|------|------|
| formate                  | NaCHO <sub>2</sub>                                                | 43.9 | 62.5  | 81.2  | 102  | 108  | 122  | 138   | 147  | 160  |
| germanate                | Na <sub>2</sub> GeO <sub>3</sub>                                  | 14.4 | 18.8  | 23.8  | 28.7 | 37.2 | 65.0 | 116   |      |      |
| hydrogen arsenate        | Na <sub>2</sub> HAsO <sub>4</sub>                                 | 5.9  | 13.0  | 33.9  | 49.3 | 69.5 | 144  | 186   | 188  | 198  |
| hydrogen carbonate       | NaHCO <sub>3</sub>                                                | 7.0  | 8.1   | 9.6   | 11.1 | 12.7 | 16.0 |       |      |      |
| hydrogen phosphate       | Na <sub>2</sub> HPO <sub>4</sub>                                  | 1.68 | 3.53  | 7.83  | 22.0 | 55.3 | 82.8 | 92.3  | 102  | 104  |
| hydrogen phosphite       | Na <sub>2</sub> HPO <sub>3</sub>                                  | 418  | 424   | 429   | 566  |      |      |       |      |      |
| hydrogen succinate       | NaC <sub>4</sub> H <sub>5</sub> O <sub>4</sub>                    | 17.5 | 25.3  | 34.8  | 47.7 | 61.6 | 74.5 | 90.1  |      |      |
| hydroxide                | NaOH                                                              |      | 98    | 109   | 119  | 129  | 174  |       |      |      |
| hydroxostannate(IV)      | Na <sub>2</sub> Sn(OH) <sub>6</sub>                               | 46.0 |       | 43.7  | 42.7 | 38.9 |      |       |      |      |
| hypochlorite             | NaClO                                                             | 29.4 | 36.4  | 53.4  | 100  | 110  |      |       |      |      |
| iodate                   | NaIO <sub>3</sub>                                                 | 2.48 | 4.59  | 8.08  | 10.7 | 13.3 | 19.8 | 26.6  | 29.5 | 33.0 |
| iodide                   | NaI                                                               | 159  | 167   | 178   | 191  | 205  | 257  | 295   |      | 302  |
| molybdate                | Na <sub>2</sub> MoO <sub>4</sub>                                  | 44.1 | 64.7  | 65.3  | 66.9 | 68.6 | 71.8 |       |      |      |
| nitrate                  | NaNO <sub>3</sub>                                                 | 73.0 | 80.8  | 87.6  | 94.9 | 102  | 122  | 148   |      | 180  |
| nitrite                  | NaNO <sub>2</sub>                                                 | 71.2 | 75.1  | 80.8  | 87.6 | 94.9 | 111  | 133   |      | 160  |
| oxalate                  | Na <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                     | 2.69 | 3.05  | 3.41  | 3.81 | 4.18 | 4.93 | 5.71  |      | 6.50 |
| perchlorate              | NaClO <sub>4</sub>                                                | 167  | 183   | 201   | 222  | 245  | 288  | 306   |      | 329  |
| periodate                | NaIO <sub>4</sub>                                                 | 1.83 | 5.6   | 10.3  | 19.9 | 30.4 |      |       |      |      |
| phosphate                | Na <sub>3</sub> PO <sub>4</sub>                                   | 4.5  | 8.2   | 12.1  | 16.3 | 20.2 | 29.9 | 60.0  | 68.1 | 77.0 |
| potassium tartrate       | NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub>                   | 31.9 | 46.6  | 67.8  | 102  |      |      |       |      |      |
| salicylate               | NaC <sub>7</sub> H <sub>5</sub> O <sub>3</sub>                    |      | 44.7  | 95.3  | 111  | 117  | 130  | 144   |      |      |
| selenate                 | Na <sub>2</sub> SeO <sub>4</sub>                                  | 13.3 | 25.2  | 26.9  | 77.0 | 81.8 | 78.6 | 74.8  | 73.0 | 72.7 |
| selenite                 | Na <sub>2</sub> SeO <sub>3</sub>                                  | 78.6 | 81.2  | 86.2  | 94.2 | 96.5 | 91.6 | 86.6  | 84.5 | 82.5 |
| sulfate                  | Na <sub>2</sub> SO <sub>4</sub>                                   | 4.9  | 9.1   | 19.5  | 40.8 | 48.8 | 45.3 | 43.7  | 42.7 | 42.5 |
|                          | Na <sub>2</sub> SO <sub>4</sub> · 7H <sub>2</sub> O               | 19.5 | 30.0  | 44.1  |      |      |      |       |      |      |
| sulfide                  | Na <sub>2</sub> S                                                 | 9.6  | 12.1  | 15.7  | 20.5 | 26.6 | 39.1 | 55.0  | 65.3 |      |
| sulfite                  | Na <sub>2</sub> SO <sub>3</sub>                                   | 14.4 | 19.5  | 26.3  | 35.5 | 37.2 | 32.6 | 29.4  | 27.9 |      |
| thioantimonate(V)        | Na <sub>3</sub> SbS <sub>4</sub>                                  | 13.4 | 20.0  | 27.9  | 37.2 | 49.3 | 53.8 | 88.3  |      |      |
| thiocyanate              | NaSCN                                                             |      | 111   | 134   | 164  | 176  | 192  | 210   | 218  |      |
| thiosulfate              | Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> · 5H <sub>2</sub> O | 50.2 | 59.7  | 70.1  | 83.2 | 104  |      |       |      |      |
| tungstate                | Na <sub>2</sub> WO <sub>4</sub>                                   | 71.5 |       | 73.0  |      | 77.6 |      | 90.8  |      | 97.2 |
| vanadate                 | NaVO <sub>3</sub>                                                 |      |       | 19.3  | 22.5 | 26.3 | 33.0 | 40.8  |      |      |
| <b>Strontium</b> acetate | Sr(C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>2</sub>    | 37.0 | 42.9  | 41.1  | 39.5 | 38.3 | 36.8 | 36.1  | 36.2 | 36.4 |
| bromide                  | SrBr <sub>2</sub>                                                 | 85.2 | 93.4  | 102   | 112  | 123  | 150  | 182   |      | 223  |
| chloride                 | SrCl <sub>2</sub>                                                 | 43.5 | 47.7  | 52.9  | 58.7 | 65.3 | 81.8 | 90.5  |      | 101  |
| chromate                 | SrCrO <sub>4</sub>                                                |      | 0.085 | 0.090 |      |      |      | 0.058 |      |      |

\*Properly called dihydrogen ethylenediaminetetraacetate (Na<sub>2</sub>H<sub>2</sub>EDTA · 2H<sub>2</sub>O).

**TABLE 5.2** Solubilities of Inorganic Compounds and Metal Salts of Organic Acids in Water at Various Temperatures (*Continued*)

| Substance                  | Formula                                                          | 0°     | 10°    | 20°    | 30°    | 40°                 | 60°    | 80°    | 90°    | 100°  |
|----------------------------|------------------------------------------------------------------|--------|--------|--------|--------|---------------------|--------|--------|--------|-------|
| <b>Strontium</b> fluoride  | SrF <sub>2</sub>                                                 | 0.0113 |        | 0.0117 | 0.0119 |                     |        |        |        |       |
| formate                    | Sr(CHO <sub>2</sub> ) <sub>2</sub>                               | 9.1    | 10.6   | 12.7   | 15.2   | 17.8                | 25.0   | 31.9   | 32.9   | 34.4  |
| hydroxide                  | Sr(OH) <sub>2</sub>                                              | 0.91   | 1.25   | 1.77   | 2.64   | 3.95                | 8.42   | 20.2   | 44.5   | 91.2  |
| iodide                     | SrI <sub>2</sub>                                                 | 165    |        | 178    |        | 192                 | 218    | 270    | 365    | 383   |
| nitrate                    | Sr(NO <sub>3</sub> ) <sub>2</sub>                                | 39.5   | 52.9   | 69.5   | 88.7   | 89.4                | 93.4   | 96.9   | 98.4   |       |
| nitrite                    | Sr(NO <sub>2</sub> ) <sub>2</sub>                                |        |        | 65     | 72     | 79                  | 97     | 130    | 134    |       |
| oxide                      | SrO                                                              |        |        |        | 1.03   | 1.05                | 3.40   | 9.15   | 13.13  | 12.15 |
| sulfate                    | SrSO <sub>4</sub>                                                | 0.0113 | 0.0129 | 0.0132 | 0.0138 | 0.0141              | 0.0131 | 0.0116 | 0.0115 |       |
| <b>Sulfamic acid</b>       | H <sub>2</sub> NSO <sub>3</sub> H                                | 14.7   | 18.6   | 21.3   | 26.1   | 29.5                | 37.1   | 47.1   |        |       |
| <b>Telluric acid</b>       | H <sub>2</sub> TeO <sub>4</sub>                                  | 16.2   | 33.8   | 41.6   | 50.0   | 57.2                | 77.5   | 106    |        | 155   |
| <b>Terbium bromate</b>     | Tb(BrO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O           | 66.4   | 89.7   | 117    | 152    | 198                 |        |        |        |       |
| <b>Thallium(I)</b> azide   | TlN <sub>3</sub>                                                 | 0.171  | 0.236  | 0.364  |        |                     |        |        |        |       |
| bromide                    | TlBr                                                             | 0.022  | 0.032  | 0.048  | 0.068  | 0.097               | 0.177  |        |        |       |
| carbonate                  | Tl <sub>2</sub> CO <sub>3</sub>                                  |        |        | 5.3    |        |                     | 12.2   |        |        | 27.2  |
| chlorate                   | TlClO <sub>3</sub>                                               | 2.00   |        | 3.92   |        | 12.7 <sup>50°</sup> |        | 36.6   |        | 57.3  |
| chloride                   | TlCl                                                             | 0.21   | 0.25   | 0.33   | 0.42   | 0.52                | 0.80   | 1.20   |        | 1.80  |
| hydroxide                  | TlOH                                                             | 25.4   | 29.6   | 35.0   | 40.4   | 49.4                | 73.3   | 106    | 126    | 150   |
| iodide                     | TlI                                                              | 0.002  |        | 0.006  |        | 0.015               | 0.035  | 0.070  |        | 0.120 |
| nitrate                    | TlNO <sub>3</sub>                                                | 3.90   | 6.22   | 9.55   | 14.3   | 21.0                | 46.1   | 110    | 200    | 414   |
| nitrite                    | TlNO <sub>2</sub>                                                | 17.9   | 28.9   | 40.3   | 53.2   | 83.6                | 216    | 1150   | 750    |       |
| perchlorate                | TlClO <sub>4</sub>                                               | 6.00   | 8.04   | 13.1   | 19.7   | 28.3                | 50.8   | 81.5   |        |       |
| picrate                    | TlOC <sub>6</sub> H <sub>2</sub> (NO <sub>2</sub> ) <sub>3</sub> | 0.135  |        | 0.40   | 0.57   | 0.83                | 1.73   |        |        |       |
| selenate                   | Tl <sub>2</sub> SeO <sub>4</sub>                                 |        | 2.17   | 2.80   |        |                     |        | 8.50   |        | 10.8  |
| sulfate                    | Tl <sub>2</sub> SO <sub>4</sub>                                  | 2.73   | 3.70   | 4.87   | 6.16   | 7.53                | 11.0   | 14.6   | 16.5   | 18.4  |
| <b>Thorium</b> nitrate     | Th(NO <sub>3</sub> ) <sub>4</sub>                                | 186    | 187    | 191    |        |                     |        |        |        |       |
| sulfate                    | Th(SO <sub>4</sub> ) <sub>2</sub> · 4H <sub>2</sub> O            |        |        |        |        | 4.04                | 1.63   |        |        |       |
|                            | Th(SO <sub>4</sub> ) <sub>2</sub> · 9H <sub>2</sub> O            | 0.74   | 0.99   | 1.38   | 1.99   | 3.00                |        |        |        |       |
| <b>Tin(II) iodide</b>      | SnI <sub>2</sub>                                                 |        |        | 0.99   | 1.17   | 1.42                | 2.11   | 3.04   | 3.58   | 4.20  |
| <b>Uranium(IV) sulfate</b> | U(SO <sub>4</sub> ) <sub>2</sub> · 4H <sub>2</sub> O             |        |        |        | 10.1   | 9.0                 | 7.7    |        |        |       |
|                            | U(SO <sub>4</sub> ) <sub>2</sub> · 8H <sub>2</sub> O             |        |        | 11.9   | 17.9   | 29.2                | 55.8   |        |        |       |

|                          |                                    |      |      |       |       |       |       |       |      |      |
|--------------------------|------------------------------------|------|------|-------|-------|-------|-------|-------|------|------|
| <b>Uranyl</b> nitrate    | $\text{UO}_2(\text{NO}_3)_2$       | 98   | 107  | 122   | 141   | 167   | 317   | 388   | 426  | 474  |
| oxalate                  | $\text{UO}_2\text{C}_2\text{O}_4$  |      | 0.45 | 0.50  | 0.61  | 0.80  | 1.22  | 1.94  |      | 3.16 |
| <b>Ytterbium sulfate</b> | $\text{Yb}_2(\text{SO}_4)_3$       | 44.2 | 37.5 |       | 22.2  | 17.2  | 10.4  | 6.4   | 5.8  | 4.7  |
| <b>Yttrium</b> bromide   | $\text{YBr}_3$                     | 63.9 |      | 75.1  |       | 87.3  | 101   | 116   | 123  |      |
| chloride                 | $\text{YCl}_3$                     | 77.3 | 78.1 | 78.8  | 79.6  | 80.8  |       |       |      |      |
| nitrate                  | $\text{Y}(\text{NO}_3)_3$          | 93.1 | 106  | 123   | 143   | 163   | 200   |       |      |      |
| sulfate                  | $\text{Y}_2(\text{SO}_4)_3$        | 8.05 | 7.67 | 7.30  | 6.78  | 6.09  | 4.44  | 2.89  | 2.2  |      |
| <b>Zinc</b> bromide      | $\text{ZnBr}_2$                    | 389  |      | 446   | 528   | 591   | 618   | 645   |      | 672  |
| chlorate                 | $\text{Zn}(\text{ClO}_3)_2$        | 145  | 152  | 200   | 209   | 223   |       |       |      |      |
| chloride                 | $\text{ZnCl}_2$                    | 342  | 363  | 395   | 437   | 452   | 488   | 541   |      | 614  |
| formate                  | $\text{Zn}(\text{CHO}_2)_2$        | 3.70 | 4.30 | 5.20  | 6.10  | 7.40  | 11.8  | 21.2  | 28.8 | 38.0 |
| iodide                   | $\text{ZnI}_2$                     | 430  |      | 432   |       | 445   | 467   | 490   |      | 510  |
| nitrate                  | $\text{Zn}(\text{NO}_3)_2$         | 98   |      |       | 138   | 211   |       |       |      |      |
| sulfate (rh)             | $\text{ZnSO}_4$                    | 41.6 | 47.2 | 53.8  | 61.3  | 70.5  | 75.4  | 71.1  |      | 60.5 |
| sulfate (mn)             |                                    |      | 54.4 | 60.0  | 65.5  |       |       |       |      |      |
| tartrate                 | $\text{ZnC}_4\text{H}_4\text{O}_6$ |      |      | 0.022 | 0.041 | 0.060 | 0.104 | 0.059 |      |      |

5.2 VAPOR PRESSURES

TABLE 5.3 Vapor Pressure of Mercury

| Temp. °C | mm of Hg  | Temp. °C | mm of Hg | Temp. °C | mm of Hg |
|----------|-----------|----------|----------|----------|----------|
| 0        | 0.000 185 | 92       | 0.1769   | 184      | 10.116   |
| 2        | 0.000 228 | 94       | 0.1976   | 186      | 10.839   |
| 4        | 0.000 276 | 96       | 0.2202   | 188      | 11.607   |
| 6        | 0.000 335 | 98       | 0.2453   | 190      | 12.423   |
| 8        | 0.000 406 | 100      | 0.2729   | 192      | 13.287   |
| 10       | 0.000 490 | 102      | 0.3032   | 194      | 14.203   |
| 12       | 0.000 588 | 104      | 0.3366   | 196      | 15.173   |
| 14       | 0.000 706 | 106      | 0.3731   | 198      | 16.200   |
| 16       | 0.000 846 | 108      | 0.4132   | 200      | 17.287   |
| 18       | 0.001 009 | 110      | 0.4572   | 202      | 18.437   |
| 20       | 0.001 201 | 112      | 0.5052   | 204      | 19.652   |
| 22       | 0.001 426 | 114      | 0.5576   | 206      | 20.936   |
| 24       | 0.001 691 | 116      | 0.6150   | 208      | 22.292   |
| 26       | 0.002 000 | 118      | 0.6776   | 210      | 23.723   |
| 28       | 0.002 359 | 120      | 0.7457   | 212      | 25.233   |
| 30       | 0.002 777 | 122      | 0.8198   | 214      | 26.826   |
| 32       | 0.003 261 | 124      | 0.9004   | 216      | 28.504   |
| 34       | 0.003 823 | 126      | 0.9882   | 218      | 30.271   |
| 36       | 0.004 471 | 128      | 1.084    | 220      | 32.133   |
| 38       | 0.005 219 | 130      | 1.186    | 222      | 34.092   |
| 40       | 0.006 079 | 132      | 1.298    | 224      | 36.153   |
| 42       | 0.007 067 | 134      | 1.419    | 226      | 38.318   |
| 44       | 0.008 200 | 136      | 1.551    | 228      | 40.595   |
| 46       | 0.009 497 | 138      | 1.692    | 230      | 42.989   |
| 48       | 0.010 98  | 140      | 1.845    | 232      | 45.503   |
| 50       | 0.012 67  | 142      | 2.010    | 234      | 48.141   |
| 52       | 0.014 59  | 144      | 2.188    | 236      | 50.909   |
| 54       | 0.016 77  | 146      | 2.379    | 238      | 53.812   |
| 56       | 0.019 25  | 148      | 2.585    | 240      | 56.855   |
| 58       | 0.022 06  | 150      | 2.807    | 242      | 60.044   |
| 60       | 0.025 24  | 152      | 3.046    | 244      | 63.384   |
| 62       | 0.028 83  | 154      | 3.303    | 246      | 66.882   |
| 64       | 0.032 87  | 156      | 3.578    | 248      | 70.543   |
| 66       | 0.037 40  | 158      | 3.873    | 250      | 74.375   |
| 68       | 0.042 51  | 160      | 4.189    | 252      | 78.381   |
| 70       | 0.048 25  | 162      | 4.528    | 254      | 82.568   |
| 72       | 0.054 69  | 164      | 4.890    | 256      | 86.944   |
| 74       | 0.061 89  | 166      | 5.277    | 258      | 91.518   |
| 76       | 0.069 93  | 168      | 5.689    | 260      | 96.296   |
| 78       | 0.078 89  | 170      | 6.128    | 262      | 101.28   |
| 80       | 0.088 80  | 172      | 6.596    | 264      | 106.48   |
| 82       | 0.100 0   | 174      | 7.095    | 266      | 111.91   |
| 84       | 0.112 4   | 176      | 7.626    | 268      | 117.57   |
| 86       | 0.126 1   | 178      | 8.193    | 270      | 123.47   |
| 88       | 0.1413    | 180      | 8.796    | 272      | 129.62   |
| 90       | 0.1582    | 182      | 9.436    | 274      | 136.02   |

**TABLE 5.3** Vapor Pressure of Mercury (*Continued*)

| Temp. °C | mm of Hg | Temp. °C | mm of Hg | Temp. °C | mm of Hg   |
|----------|----------|----------|----------|----------|------------|
| 276      | 142.69   | 332      | 478.13   | 388      | 1299.1     |
| 278      | 149.64   | 334      | 497.12   | 390      | 1341.9     |
| 280      | 156.87   | 336      | 516.74   | 392      | 1386.1     |
| 282      | 164.39   | 338      | 537.00   | 394      | 1431.3     |
| 284      | 172.21   | 340      | 557.90   | 396      | 1477.7     |
| 286      | 180.34   | 342      | 579.45   | 398      | 1525.2     |
| 288      | 188.79   | 344      | 601.69   | 400      | 1574.1     |
| 290      | 197.57   | 346      | 624.64   | 430      | 2464       |
| 292      | 206.70   | 348      | 648.30   | 460      | 3715       |
| 294      | 216.17   | 350      | 672.69   | 490      | 5420       |
| 296      | 226.00   | 352      | 697.83   | 520      | 7691       |
| 298      | 236.21   | 354      | 723.73   | 550      | 10650      |
| 300      | 246.80   | 356      | 750.43   | 600      | 22.87 atm  |
| 302      | 257.78   | 358      | 777.92   | 650      | 35.49 atm  |
| 304      | 269.17   | 360      | 806.23   | 700      | 52.51 atm  |
| 306      | 280.98   | 362      | 835.38   | 750      | 74.86 atm  |
| 308      | 293.21   | 364      | 865.36   | 800      | 103.31 atm |
| 310      | 305.89   | 366      | 896.23   | 850      | 138.42 atm |
| 312      | 319.02   | 368      | 928.02   | 900*     | 180.92 atm |
| 314      | 332.62   | 370      | 960.66   | 950      | 226.58 atm |
| 316      | 346.70   | 372      | 994.34   | 1000     | 290.5 atm  |
| 318      | 361.26   | 374      | 1028.9   | 1050     | 358.1 atm  |
| 320      | 376.33   | 376      | 1064.4   | 1100     | 437.3 atm  |
| 322      | 391.92   | 378      | 1100.9   | 1150     | 521.3 atm  |
| 324      | 408.04   | 380      | 1138.4   | 1200     | 616.8 atm  |
| 326      | 424.71   | 382      | 1177.0   | 1250     | 721.4 atm  |
| 328      | 441.94   | 384      | 1216.6   | 1300     | 835.9 atm  |
| 330      | 459.74   | 386      | 1257.3   |          |            |

\* Critical point.

**TABLE 5.4** Vapor Pressure of Ice in Millimeters of Mercury

For temperatures from  $-99$  to  $0^{\circ}\text{C}$ .

The values in the table are for ice in contact with its own vapor. Where the ice is in contact with air at a temperature  $t^{\circ}\text{C}$ , this correction must be added:  $\text{Correction} = 20p/(100)(t + 273)$ .

| $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ | $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ | $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ |
|-----------------------|--------------------|-----------------------|--------------------|-----------------------|--------------------|
| -99                   | 0.000 012          | -51                   | 0.026 1            | -16.5                 | 1.080              |
| -98                   | 0.000 015          | -50                   | 0.029 6            | -16.0                 | 1.132              |
| -97                   | 0.000 018          | -49                   | 0.033 4            | -15.5                 | 1.186              |
| -96                   | 0.000 022          | -48                   | 0.037 8            | -15.0                 | 0.241              |
| -95                   | 0.000 027          | -47                   | 0.042 6            | -14.5                 | 1.300              |
| -94                   | 0.000 033          | -46                   | 0.048 1            | -14.0                 | 1.361              |
| -93                   | 0.000 040          | -45                   | 0.054 1            | -13.5                 | 1.424              |
| -92                   | 0.000 048          | -44                   | 0.060 9            | -13.0                 | 1.490              |
| -91                   | 0.000 058          | -43                   | 0.068 4            | -12.5                 | 1.559              |
| -90                   | 0.000 070          | -42                   | 0.076 8            | -12.0                 | 1.632              |
| -89                   | 0.000 084          | -41                   | 0.086 2            | -11.5                 | 1.707              |
| -88                   | 0.000 10           | -40                   | 0.096 6            | -11.0                 | 1.785              |
| -87                   | 0.000 12           | -39                   | 0.108 1            | -10.5                 | 1.866              |
| -86                   | 0.000 14           | -38                   | 0.120 9            | -10.0                 | 1.950              |
| -85                   | 0.000 17           | -37                   | 0.135 1            | -9.8                  | 1.985              |
| -84                   | 0.000 20           | -36                   | 0.150 7            | -9.6                  | 2.021              |
| -83                   | 0.000 24           | -35                   | 0.168 1            | -9.4                  | 2.057              |
| -82                   | 0.000 29           | -34                   | 0.187 3            | -9.2                  | 2.093              |
| -81                   | 0.000 34           | -33                   | 0.208 4            | -9.0                  | 2.131              |
| -80                   | 0.000 40           | -32                   | 0.231 8            | -8.8                  | 2.168              |
| -79                   | 0.000 47           | -31                   | 0.257 5            | -8.6                  | 2.207              |
| -78                   | 0.000 56           | -30.0                 | 0.285 9            | -8.4                  | 2.246              |
| -77                   | 0.000 66           | -29.5                 | 0.301              | -8.2                  | 2.285              |
| -76                   | 0.000 77           | -29.0                 | 0.317              | -8.0                  | 2.326              |
| -75                   | 0.000 90           | -28.5                 | 0.334              | -7.8                  | 2.367              |
| -74                   | 0.001 05           | -28.0                 | 0.351              | -7.6                  | 2.408              |
| -73                   | 0.001 23           | -27.5                 | 0.370              | -7.4                  | 2.450              |
| -72                   | 0.001 43           | -27.0                 | 0.389              | -7.2                  | 2.493              |
| -71                   | 0.001 67           | -26.5                 | 0.409              | -7.0                  | 2.537              |
| -70                   | 0.001 94           | -26.0                 | 0.430              | -6.8                  | 2.581              |
| -69                   | 0.002 25           | -25.5                 | 0.453              | -6.6                  | 2.626              |
| -68                   | 0.002 61           | -25.0                 | 0.476              | -6.4                  | 2.672              |
| -67                   | 0.003 02           | -24.5                 | 0.500              | -6.2                  | 2.718              |
| -66                   | 0.003 49           | -24.0                 | 0.526              | -6.0                  | 2.765              |
| -65                   | 0.004 03           | -23.5                 | 0.552              | -5.8                  | 2.813              |
| -64                   | 0.004 64           | -23.0                 | 0.580              | -5.6                  | 2.862              |
| -63                   | 0.005 34           | -22.5                 | 0.609              | -5.4                  | 2.912              |
| -62                   | 0.006 14           | -22.0                 | 0.640              | -5.2                  | 2.962              |
| -61                   | 0.007 03           | -21.5                 | 0.672              | -5.0                  | 3.013              |
| -60                   | 0.008 08           | -21.0                 | 0.705              | -4.8                  | 3.065              |
| -59                   | 0.009 25           | -20.5                 | 0.740              | -4.6                  | 3.117              |
| -58                   | 0.010 6            | -20.0                 | 0.776              | -4.4                  | 3.171              |
| -57                   | 0.012 1            | -19.5                 | 0.814              | -4.2                  | 3.225              |
| -56                   | 0.013 8            | -19.0                 | 0.854              | -4.0                  | 3.280              |
| -55                   | 0.015 7            | -18.5                 | 0.895              | -3.8                  | 3.336              |
| -54                   | 0.017 8            | -18.0                 | 0.939              | -3.6                  | 3.393              |
| -53                   | 0.020 3            | -17.5                 | 0.984              | -3.4                  | 3.451              |
| -52                   | 0.023 0            | -17.0                 | 1.031              | -3.2                  | 3.509              |

**TABLE 5.4** Vapor Pressure of Ice in Millimeters of Mercury (*Continued*)

| <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg |
|---------------|------------------|---------------|------------------|---------------|------------------|
| −3.0          | 3.568            | −1.8          | 3.946            | −0.8          | 4.287            |
| −2.8          | 3.360            | −1.6          | 4.012            | −0.6          | 4.359            |
| −2.6          | 3.691            | −1.4          | 4.079            | −0.4          | 4.431            |
| −2.4          | 3.753            | −1.2          | 4.147            | −0.2          | 4.504            |
| −2.2          | 3.816            | −1.0          | 4.217            | 0.0           | 4.579            |
| −2.0          | 3.880            |               |                  |               |                  |

**TABLE 5.5** Vapor Pressure of Liquid Ammonia, NH<sub>3</sub>

| <i>t</i> °C. | <i>p</i> in atm | <i>t</i> °C. | <i>p</i> in atm | <i>t</i> °C. | <i>p</i> in atm |
|--------------|-----------------|--------------|-----------------|--------------|-----------------|
| −78          | 0.0582          | −6           | 3.3677          | 66           | 29.784          |
| −76          | 0.0683          | −4           | 3.6405          | 68           | 31.211          |
| −74          | 0.0797          | −2           | 3.9303          | 70           | 32.687          |
| −72          | 0.0929          | 0            | 4.2380          | 72           | 34.227          |
| −70          | 0.1078          | +2           | 4.5640          | 74           | 35.813          |
| −68          | 0.1246          | 4            | 4.9090          | 76           | 37.453          |
| −66          | 0.1437          | 6            | 5.2750          | 78           | 39.149          |
| −64          | 0.1651          | 8            | 5.6610          | 80           | 40.902          |
| −62          | 0.1891          | 10           | 6.0685          | 82           | 42.712          |
| −60          | 0.2161          | 12           | 6.4985          | 84           | 44.582          |
| −58          | 0.2461          | 14           | 6.9520          | 86           | 46.511          |
| −56          | 0.2796          | 16           | 7.4290          | 88           | 48.503          |
| −54          | 0.3167          | 18           | 7.9310          | 90           | 50.558          |
| −52          | 0.3578          | 20           | 8.4585          | 92           | 52.677          |
| −50          | 0.4034          | 22           | 9.0125          | 94           | 54.860          |
| −48          | 0.4536          | 24           | 9.5940          | 96           | 57.111          |
| −46          | 0.5087          | 26           | 10.2040         | 98           | 59.429          |
| −44          | 0.5693          | 28           | 10.8430         | 100          | 61.816          |
| −42          | 0.6357          | 30           | 11.512          | 102          | 64.274          |
| −40          | 0.7083          | 32           | 12.212          | 104          | 66.804          |
| −38          | 0.7875          | 34           | 12.943          | 106          | 69.406          |
| −36          | 0.8738          | 36           | 13.708          | 108          | 72.084          |
| −34          | 0.9676          | 38           | 14.507          | 110          | 74.837          |
| −32          | 1.0695          | 40           | 15.339          | 112          | 77.668          |
| −30          | 1.1799          | 42           | 16.209          | 114          | 80.578          |
| −28          | 1.2992          | 44           | 17.113          | 116          | 83.570          |
| −26          | 1.4281          | 46           | 18.056          | 118          | 86.644          |
| −24          | 1.5671          | 48           | 19.038          | 120          | 89.802          |
| −22          | 1.7166          | 50           | 20.059          | 122          | 93.045          |
| −20          | 1.8774          | 52           | 21.121          | 124          | 96.376          |
| −18          | 2.0499          | 54           | 22.224          | 126          | 99.796          |
| −16          | 2.2349          | 56           | 23.372          | 128          | 103.309         |
| −14          | 2.4328          | 58           | 24.562          | 130          | 106.913         |
| −12          | 2.6443          | 60           | 25.797          | 132          | 110.613         |
| −10          | 2.8703          | 62           | 27.079          | 132.3        | 111.3(c.p.)     |
| −8           | 3.1112          | 64           | 28.407          |              |                 |



**TABLE 5.6** Vapor Pressure of Water

For temperatures from  $-10$  to  $120^{\circ}\text{C}$ .

The values in the table are for water in contact with its own vapor. Where the water is in contact with air at a temperature  $t$  in degrees Celsius, the following correction must be added: Correction (when  $t \leq 40^{\circ}\text{C}$ ) =  $p(0.775 - 0.000\,313t)/100$ ; correction (when  $t > 50^{\circ}\text{C}$ ) =  $p(0.0652 - 0.000\,087\,5t)/100$ .

| $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ | $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ | $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ | $t, ^{\circ}\text{C}$ | $p, \text{ mm Hg}$ |
|-----------------------|--------------------|-----------------------|--------------------|-----------------------|--------------------|-----------------------|--------------------|
| -10.0                 | 2.149              | 13.0                  | 11.231             | 23.4                  | 21.583             | 32.6                  | 36.891             |
| -9.5                  | 2.236              | 13.5                  | 11.604             | 23.6                  | 21.845             | 32.8                  | 37.308             |
| -9.0                  | 2.326              | 14.0                  | 11.987             | 23.8                  | 22.110             | 33.0                  | 37.729             |
| -8.5                  | 2.418              | 14.5                  | 12.382             | 24.0                  | 22.387             | 33.2                  | 38.155             |
| -8.0                  | 2.514              | 15.0                  | 12.788             | 24.2                  | 22.648             | 33.4                  | 38.584             |
| -7.5                  | 2.613              | 15.2                  | 12.953             | 24.4                  | 22.922             | 33.6                  | 39.018             |
| -7.0                  | 2.715              | 15.4                  | 13.121             | 24.6                  | 23.198             | 33.8                  | 39.457             |
| -6.5                  | 2.822              | 15.6                  | 13.290             | 24.8                  | 23.476             | 34.0                  | 39.898             |
| -6.0                  | 2.931              | 15.8                  | 13.461             | 25.0                  | 23.756             | 34.2                  | 40.344             |
| -5.5                  | 3.046              | 16.0                  | 13.634             | 25.2                  | 24.039             | 34.4                  | 40.796             |
| -5.0                  | 3.163              | 16.2                  | 13.809             | 25.4                  | 24.326             | 34.6                  | 41.251             |
| -4.5                  | 3.284              | 16.4                  | 13.987             | 25.6                  | 24.617             | 34.8                  | 41.710             |
| -4.0                  | 3.410              | 16.6                  | 14.166             | 25.8                  | 24.912             | 35.0                  | 42.175             |
| -3.5                  | 3.540              | 16.8                  | 14.347             | 26.0                  | 25.209             | 35.2                  | 42.644             |
| -3.0                  | 3.673              | 17.0                  | 14.530             | 26.2                  | 25.509             | 35.4                  | 43.117             |
| -2.5                  | 3.813              | 17.2                  | 14.715             | 26.4                  | 25.812             | 35.6                  | 43.595             |
| -2.0                  | 3.956              | 17.4                  | 14.903             | 26.6                  | 26.117             | 35.8                  | 44.078             |
| -1.5                  | 4.105              | 17.6                  | 15.092             | 26.8                  | 26.426             | 36.0                  | 44.563             |
| -1.0                  | 4.258              | 17.8                  | 15.284             | 27.0                  | 26.739             | 36.2                  | 45.054             |
| -0.5                  | 4.416              | 18.0                  | 15.477             | 27.2                  | 27.055             | 36.4                  | 45.549             |
| 0.0                   | 4.579              | 18.2                  | 15.673             | 27.4                  | 27.374             | 36.6                  | 46.050             |
| 0.5                   | 4.750              | 18.4                  | 15.871             | 27.6                  | 27.696             | 36.8                  | 46.556             |
| 1.0                   | 4.926              | 18.6                  | 16.071             | 27.8                  | 28.021             | 37.0                  | 47.067             |
| 1.5                   | 5.107              | 18.8                  | 16.272             | 28.0                  | 28.349             | 37.2                  | 47.582             |
| 2.0                   | 5.294              | 19.0                  | 16.477             | 28.2                  | 28.680             | 37.4                  | 48.102             |
| 2.5                   | 5.486              | 19.2                  | 16.685             | 28.4                  | 29.015             | 37.6                  | 48.627             |
| 3.0                   | 5.685              | 19.4                  | 16.894             | 28.6                  | 29.354             | 37.8                  | 49.157             |
| 3.5                   | 5.889              | 19.6                  | 17.105             | 28.8                  | 29.697             | 38.0                  | 49.692             |
| 4.0                   | 6.101              | 19.8                  | 17.319             | 29.0                  | 30.043             | 38.2                  | 50.231             |
| 4.5                   | 6.318              | 20.0                  | 17.535             | 29.2                  | 30.392             | 38.4                  | 50.774             |
| 5.0                   | 6.543              | 20.2                  | 17.753             | 29.4                  | 30.745             | 38.6                  | 51.323             |
| 5.5                   | 6.775              | 20.4                  | 17.974             | 29.6                  | 31.102             | 38.8                  | 51.879             |
| 6.0                   | 7.013              | 20.6                  | 18.197             | 29.8                  | 31.461             | 39.0                  | 52.442             |
| 6.5                   | 7.259              | 20.8                  | 18.422             | 30.0                  | 31.824             | 39.2                  | 53.009             |
| 7.0                   | 7.513              | 21.0                  | 18.650             | 30.2                  | 32.191             | 39.4                  | 54.580             |
| 7.5                   | 7.775              | 21.2                  | 18.880             | 30.4                  | 32.561             | 39.6                  | 54.156             |
| 8.0                   | 8.045              | 21.4                  | 19.113             | 30.6                  | 32.934             | 39.8                  | 54.737             |
| 8.5                   | 8.323              | 21.6                  | 19.349             | 30.8                  | 33.312             | 40.0                  | 55.324             |
| 9.0                   | 8.609              | 21.8                  | 19.587             | 31.0                  | 33.695             | 40.5                  | 56.81              |
| 9.5                   | 8.905              | 22.0                  | 19.827             | 31.2                  | 34.082             | 41.0                  | 58.34              |
| 10.0                  | 9.209              | 22.2                  | 20.070             | 31.4                  | 34.471             | 41.5                  | 59.90              |
| 10.5                  | 9.521              | 22.4                  | 20.316             | 31.6                  | 34.864             | 42.0                  | 61.50              |
| 11.0                  | 9.844              | 22.6                  | 20.565             | 31.8                  | 35.261             | 42.5                  | 63.13              |
| 11.5                  | 10.176             | 22.8                  | 20.815             | 32.0                  | 35.663             | 43.0                  | 64.80              |
| 12.0                  | 10.518             | 23.0                  | 21.068             | 32.2                  | 36.068             | 43.5                  | 66.51              |
| 12.5                  | 10.870             | 23.2                  | 21.324             | 32.4                  | 36.477             | 44.0                  | 68.26              |

TABLE 5.6 Vapor Pressure of Water (Continued)

| <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg |
|---------------|------------------|---------------|------------------|---------------|------------------|---------------|------------------|
| 44.5          | 70.05            | 63.0          | 171.38           | 81.5          | 377.3            | 97.0          | 682.07           |
| 45.0          | 71.88            | 63.5          | 175.35           | 82.0          | 384.9            | 97.2          | 687.04           |
| 45.5          | 73.74            | 64.0          | 179.31           | 82.5          | 392.8            | 97.4          | 692.05           |
| 46.0          | 75.65            | 64.5          | 183.43           | 83.0          | 400.6            | 97.6          | 697.10           |
| 46.5          | 77.61            | 65.0          | 187.54           | 83.5          | 408.7            | 97.8          | 702.17           |
| 47.0          | 79.60            | 65.5          | 191.82           | 84.0          | 416.8            | 98.0          | 707.27           |
| 47.5          | 81.64            | 66.0          | 196.09           | 84.5          | 425.2            | 98.2          | 712.40           |
| 48.0          | 83.71            | 66.5          | 200.53           | 85.0          | 433.6            | 98.4          | 717.56           |
| 48.5          | 85.85            | 67.0          | 204.96           | 85.5          | 442.3            | 98.6          | 722.75           |
| 49.0          | 88.02            | 67.5          | 209.57           | 86.0          | 450.9            | 98.8          | 727.98           |
| 49.5          | 90.24            | 68.0          | 214.17           | 86.5          | 459.8            | 99.0          | 733.24           |
| 50.0          | 92.51            | 68.5          | 218.95           | 87.0          | 468.7            | 99.2          | 738.53           |
| 50.5          | 94.86            | 69.0          | 223.73           | 87.5          | 477.9            | 99.4          | 743.85           |
| 51.0          | 97.20            | 69.5          | 228.72           | 88.0          | 487.1            | 99.6          | 749.20           |
| 51.5          | 99.65            | 70.0          | 233.7            | 88.5          | 496.6            | 99.8          | 754.58           |
| 52.0          | 102.09           | 70.5          | 238.8            | 89.0          | 506.1            | 100.0         | 760.00           |
| 52.5          | 104.65           | 71.0          | 243.9            | 89.5          | 515.9            | 101.0         | 787.57           |
| 53.0          | 107.20           | 71.5          | 249.3            | 90.0          | 525.76           | 102.0         | 815.86           |
| 53.5          | 109.86           | 72.0          | 254.6            | 90.5          | 535.83           | 103.0         | 845.12           |
| 54.0          | 112.51           | 72.5          | 260.2            | 91.0          | 546.05           | 104.0         | 875.06           |
| 54.5          | 115.28           | 73.0          | 265.7            | 91.5          | 556.44           | 105.0         | 906.07           |
| 55.0          | 118.04           | 73.5          | 271.5            | 92.0          | 566.99           | 106.0         | 937.92           |
| 55.5          | 120.92           | 74.0          | 277.2            | 92.5          | 577.71           | 107.0         | 970.60           |
| 56.0          | 123.80           | 74.5          | 283.2            | 93.0          | 588.60           | 108.0         | 1004.42          |
| 56.5          | 126.81           | 75.0          | 289.1            | 93.5          | 599.66           | 109.0         | 1038.92          |
| 57.0          | 129.82           | 75.5          | 295.3            | 94.0          | 610.90           | 110.0         | 1074.56          |
| 57.5          | 132.95           | 76.0          | 301.4            | 94.5          | 622.31           | 111.0         | 1111.20          |
| 58.0          | 136.08           | 76.5          | 307.7            | 95.0          | 633.90           | 112.0         | 1148.74          |
| 58.5          | 139.34           | 77.0          | 314.1            | 95.2          | 638.59           | 113.0         | 1187.42          |
| 59.0          | 142.60           | 77.5          | 320.7            | 95.4          | 643.30           | 114.0         | 1227.25          |
| 59.5          | 145.99           | 78.0          | 327.3            | 95.6          | 648.05           | 115.0         | 1267.98          |
| 60.0          | 149.38           | 78.5          | 334.2            | 95.8          | 652.82           | 116.0         | 1309.94          |
| 60.5          | 152.91           | 79.0          | 341.0            | 96.0          | 657.62           | 117.0         | 1352.95          |
| 61.0          | 156.43           | 79.5          | 348.1            | 96.2          | 662.45           | 118.0         | 1397.18          |
| 61.5          | 160.10           | 80.0          | 355.1            | 96.4          | 667.31           | 119.0         | 1442.63          |
| 62.0          | 163.77           | 80.5          | 362.4            | 96.6          | 672.20           | 120.0         | 1489.14          |
| 62.5          | 167.58           | 81.0          | 369.7            | 96.8          | 677.12           |               |                  |

TABLE 5.7 Vapor Pressure of Deuterium Oxide

| <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg | <i>t</i> , °C | <i>p</i> , mm Hg |
|---------------|------------------|---------------|------------------|---------------|------------------|
| 0             | 3.65             | 20            | 15.2             | 80            | 331.6            |
| 1             | 3.93             | 30            | 28.0             | 90            | 495.5            |
| 2             | 4.29             | 40            | 49.3             | 100           | 722.2            |
| 3             | 4.65             | 50            | 83.6             | 101.43        | 760.0            |
| 3.8           | 5.05             | 60            | 136.6            |               |                  |
| 10            | 7.79             | 70            | 216.1            |               |                  |

5.2.1 Vapor-Pressure Equations

Numerous mathematical formulas relating the temperature and pressure of the gas phase in equilibrium with the condensed phase have been proposed. The Antoine equation (Eq. 1) gives good correlation with experimental values. Equation 2 is simpler and is often suitable over restricted temperature ranges. In these equations, and the derived differential coefficients for use in the Hagenmacher and Clausius-Clapeyron equations, the  $p$  term is the vapor pressure of the compound in pounds per square inch (psi), the  $t$  term is the temperature in degrees Celsius, and the  $T$  term is the absolute temperature in kelvins ( $t^{\circ}\text{C} + 273.15$ ).

| Eq. | Vapor-pressure equation               | $dp/dT$                                             | $-[d(\ln p)/d(1/T)]$          |
|-----|---------------------------------------|-----------------------------------------------------|-------------------------------|
| 1   | $\log p = A - \frac{B}{t + C}$        | $\frac{2.303pB}{(t + C)^2}$                         | $\frac{2.303BT^2}{(t + C)^2}$ |
| 2   | $\log p = A - \frac{B}{T}$            | $\frac{2.303pB}{T^2}$                               | $2.303B$                      |
| 3   | $\log p = A - \frac{B}{T} - C \log T$ | $p \left( \frac{2.303B}{T^2} - \frac{C}{T} \right)$ | $2.303B - CT$                 |

Equations 1 and 2 are easily rearranged to calculate the temperature of the normal boiling point:

$$t = \frac{B}{A - \log p} - C \tag{5.1}$$

$$T = \frac{B}{A - \log p} \tag{5.2}$$

The constants in the Antoine equation may be estimated by selecting three widely spaced data points and substituting in the following equations in sequence:

$$\left(\frac{y_3 - y_2}{y_2 - y_1}\right)\left(\frac{t_2 - t_1}{t_3 - t_2}\right) = 1 - \left(\frac{t_3 - t_1}{t_3 + C}\right)$$

$$B = \left(\frac{y_3 - y_1}{t_3 - t_1}\right)(t_1 + C)(t_3 + C)$$

$$A = y_2 + \left(\frac{B}{t_2 + C}\right)$$

In these equations,  $y_i = \log p_i$ .

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds

| Substance                        | State  | Eq. | Range, °C   | A        | B         | C      |
|----------------------------------|--------|-----|-------------|----------|-----------|--------|
| <b>Aluminum</b>                  |        |     |             |          |           |        |
| AlCl <sub>3</sub>                |        | 2   | 70–190      | 16.24    | 6 006     |        |
| Al <sub>2</sub> O <sub>3</sub>   |        | 2   | 1840–2000   | 14.22    | 28 200    |        |
| <b>Ammonium</b>                  |        |     |             |          |           |        |
| NH <sub>3</sub>                  | c*     | 1   |             | 9.963 82 | 1 617.907 | 272.55 |
|                                  | liq    | 1   |             | 7.360 50 | 926.132   | 240.17 |
| NH <sub>4</sub> Br               | subl c | 1   |             | 9.220 0  | 3 947     | 227.0  |
| NH <sub>4</sub> Cl               | subl c | 1   |             | 9.355 7  | 3 703.7   | 232.0  |
| NH <sub>4</sub> I                | subl c | 1   |             | 9.147 0  | 3 858     | 226.0  |
| NH <sub>4</sub> N <sub>3</sub>   | c      | 1   |             | 10.433 4 | 2 821.0   | 240.0  |
| <b>Antimony</b>                  |        |     |             |          |           |        |
| Sb                               | c      | 2   | 1070–1325   | 9.051    | 9 871     |        |
| SbBr <sub>3</sub>                |        | 2   | 235–324     | 8.005    | 2 873     |        |
| SbCl <sub>3</sub>                |        | 2   | 170–253     | 8.090    | 2 582.3   |        |
| SbI <sub>3</sub>                 |        | 2   | 330–445     | 7.831    | 3 350.55  |        |
| Sb <sub>2</sub> Se <sub>3</sub>  | subl c | 2   |             | 8.790 6  | 6 432.3   |        |
| <b>Argon</b>                     |        |     |             |          |           |        |
| Ar                               | c      | 1   |             | 7.505 81 | 399.085   | 272.63 |
|                                  | liq    | 1   |             | 6.616 51 | 304.227   | 267.32 |
| <b>Arsenic</b>                   |        |     |             |          |           |        |
| As                               |        | 2   | 440–815     | 10.800   | 6 947     |        |
|                                  |        | 2   | 800–860     | 6.692    | 2 460     |        |
| AsCl <sub>3</sub>                |        | 2   | 50–100      | 7.953    | 2 042.7   |        |
| As <sub>2</sub> O <sub>3</sub>   |        | 2   | 100–310     | 12.127   | 5 815.81  |        |
|                                  |        | 2   | 315–490     | 6.513    | 2 722.2   |        |
| <b>Barium</b>                    |        |     |             |          |           |        |
| Ba                               |        | 2   | 930–1130    | 15.765   | 18 280    |        |
| BaH <sub>2</sub> [97% pure]      |        | 2   | 500–1000    | 6.86     | 4 000     |        |
| <b>Bismuth</b>                   |        |     |             |          |           |        |
| Bi                               |        | 2   | 1210–1420   | 8.876    | 10 446    |        |
| BiCl <sub>3</sub>                |        | 2   | 91–213      | 2.681    | 685.519   |        |
| <b>Boron</b>                     |        |     |             |          |           |        |
| BBr <sub>3</sub>                 |        | 2   | –40 to 90   | 7.655    | 1 740.3   |        |
| BCl <sub>3</sub>                 |        | 1   |             | 6.188 11 | 756.89    | 214.0  |
| B(CH <sub>3</sub> ) <sub>3</sub> |        | 2   | –118 to –20 | 7.459 5  | 1 157.99  |        |
| B <sub>2</sub> H <sub>6</sub>    | liq    | 1   |             | 6.366 38 | 521.490   | 241.98 |
| B <sub>5</sub> H <sub>11</sub>   | liq    | 2   | –43 to 8.4  | 7.901    | 1 690.3   |        |
| <b>Bromine</b>                   |        |     |             |          |           |        |
| Br <sub>2</sub>                  | c      | 1   |             | 9.7209   | 2 041.3   | 260.1  |
|                                  | liq    | 1   |             | 6.877 80 | 1 119.68  | 221.38 |
| BrF <sub>3</sub>                 | liq    | 1   |             | 7.729 74 | 1 673.95  | 219.48 |
| BrF <sub>5</sub>                 | liq    | 1   |             | 7.273 68 | 1 219.28  | 236.40 |
| BrO <sub>2</sub> F               | liq    | 1   |             | 7.436 51 | 1 195.8   | 260.1  |
| <b>Cadmium</b>                   |        |     |             |          |           |        |
| Cd                               |        | 2   | 150–321     | 8.564    | 5 693     |        |
|                                  |        | 2   | 500–840     | 7.897    | 5 218     |        |
|                                  |        | 2   | 385–450     | 9.269    | 6 383     |        |
| <b>Calcium</b>                   |        |     |             |          |           |        |
| Ca                               |        | 2   | 500–700     | 9.697    | 10 185    |        |
|                                  |        | 2   | 960–1100    | 16.240   | 19 325    |        |

\* Crystalline solid.

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                      | State  | Eq. | Range, °C            | A        | B         | C       |
|--------------------------------|--------|-----|----------------------|----------|-----------|---------|
| <b>Carbon</b>                  |        |     |                      |          |           |         |
| C [as C(g)]                    | liq    | 1   |                      | 11.042 8 | 37 736    | 302.2   |
| [as C <sub>2</sub> (g)]        | liq    | 1   |                      | 12.583 2 | 43 281    | 318.3   |
| [all species]                  | liq    | 1   |                      | 9.381 3  | 27 240    | 264.0   |
| <b>Carbon</b>                  |        |     |                      |          |           |         |
| CNBr                           | subl c | 1   |                      | 9.488 9  | 2 041.8   | 251.70  |
| CNF                            |        | 1   | − 76 to − 47         | 6.778 9  | 697.61    | 224.95  |
| CO                             | c I    | 1   |                      | 7.414 8  | 342.50    | 269.0   |
|                                | liq    | 1   |                      | 6.694 22 | 291.743   | 267.99  |
| CO <sub>2</sub>                | c      | 1   |                      | 9.810 66 | 1 347.786 | 273.00  |
| C <sub>3</sub> O <sub>2</sub>  | liq    | 1   | − 71 to 7            | 7.188 99 | 1 100.94  | 249.15  |
| COCl <sub>2</sub>              | liq    | 1   |                      | 6.971 33 | 998.770   | 236.68  |
| COF <sub>2</sub>               |        | 1   | − 109 to − 84        | 6.885 5  | 576.70    | 228.58  |
| COS                            |        | 1   | − 111 to − 49        | 6.907 23 | 804.48    | 250.0   |
| CS <sub>2</sub>                |        | 1   | 3–80                 | 6.942 79 | 1 169.11  | 241.59  |
| CSe <sub>2</sub>               |        | 1   | 0–50                 | 6.776 73 | 1 353.20  | 219.95  |
| CSeS                           |        | 1   | − 16 to 84           | 6.699 6  | 1 161.97  | 219.59  |
| <b>Cesium</b>                  |        |     |                      |          |           |         |
| Cs                             |        | 2   | 200–350              | 6.949    | 3 833.7   |         |
| CsBr                           |        | 2   | 978–1305             | 7.990    | 8 022.53  |         |
| CsCl                           |        | 2   | 986–1295             | 8.340    | 8 523.94  |         |
| CsF                            |        | 2   | 1033–1255            | 7.703    | 7 359.21  |         |
| CsH                            |        | 2   | 245–378              | 11.79    | 5 900     |         |
|                                |        | 2   | 340–440              | 9.25     | 4 410     |         |
| CsI                            |        | 2   | 1052–1280            | 9.124    | 9 699.11  |         |
| <b>Chlorine</b>                |        |     |                      |          |           |         |
| Cl <sub>2</sub>                | c      | 1   |                      | 9.705 12 | 1 444.19  | 267.13  |
|                                | liq    | 1   |                      | 6.937 90 | 861.34    | 246.33  |
| ClF                            | liq    | 1   |                      | 6.989    | 682.1     | 256     |
| ClF <sub>3</sub>               | liq    | 1   |                      | 7.366 85 | 1 096.28  | 232.63  |
| ClF <sub>5</sub>               |        | 1   |                      | 6.269 33 | 653.06    | 206.6   |
| ClO <sub>2</sub>               | liq    | 1   |                      | 6.036 11 | 590.09    | 176.15  |
| Cl <sub>2</sub> O              | liq    | 1   |                      | 7.132 68 | 1 021.56  | 238.16  |
| ClOClO <sub>3</sub>            | liq    | 1   |                      | 7.538 67 | 1 404.18  | 257.00  |
| Cl <sub>2</sub> O <sub>7</sub> | liq    | 1   |                      | 6.869 29 | 1 214.00  | 220.79  |
| ClO <sub>2</sub> F             | liq    | 1   |                      | 6.677 15 | 809.78    | 218.96  |
| ClO <sub>3</sub> F             | liq    | 1   |                      | 6.895 19 | 791.73    | 243.88  |
| <b>Copper</b>                  |        |     |                      |          |           |         |
| CuBr                           |        | 2   | 997–1351             | 5.460    | 4 173.2   |         |
| CuCl                           |        | 2   | 878–1369             | 5.454    | 4 215.0   |         |
| CuI                            |        | 2   | 991–1154             | 5.570    | 4 215.0   |         |
| <b>Fluorine</b>                |        |     |                      |          |           |         |
| F <sub>2</sub>                 | liq    | 1   |                      | 6.765 88 | 304.35    | 266.54  |
| FNO <sub>3</sub>               | liq    | 1   |                      | 6.658 6  | 769.5     | 248.0   |
| <b>Germanium</b>               |        |     |                      |          |           |         |
| GeCl <sub>4</sub>              |        | 2   | 10.4–86              | 7.340    | 2 010.9   |         |
| <b>Helium</b>                  |        |     |                      |          |           |         |
| <sup>3</sup> He                | liq    | 1   | − 271.13 to − 270.86 | 4.272 7  | 5.594     | 273.840 |
|                                | liq    | 1   | − 271.13 to − 269.92 | 5.100 0  | 11.062    | 274.950 |
| <sup>4</sup> He                |        | 1   | − 271.4 to − 270.1   | 4.558 7  | 8.1548    | 273.710 |
|                                |        | 1   | − 271.4 to − 268.9   | 5.320 75 | 14.6515   | 274.950 |
|                                |        | 1   | − 271.4 to − 268.1   | 6.004 60 | 24.0668   | 276.650 |

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                                                            | State | Eq. | Range, °C  | A                        | B        | C       |
|----------------------------------------------------------------------|-------|-----|------------|--------------------------|----------|---------|
| <b>Hydrogen</b>                                                      |       |     |            |                          |          |         |
| <sup>1</sup> H <sub>2</sub> normal, 25% para<br>equilibrium          | c     | 1   |            | 6.043 86                 | 66.507   | 274.630 |
|                                                                      | liq   | 1   |            | 5.824 38                 | 67.5078  | 275.700 |
|                                                                      | c     | 1   |            | 6.042 07                 | 65.961   | 274.60  |
|                                                                      | liq   | 1   |            | 5.814 64                 | 66.7945  | 275.650 |
| <sup>1</sup> H <sup>2</sup> H (DH)                                   | c     | 1   |            | 6.960 08                 | 99.968   | 276.590 |
|                                                                      | liq   | 1   |            | 6.016 12                 | 77.1349  | 275.620 |
| <sup>2</sup> H <sub>2</sub> (D <sub>2</sub> ) normal,<br>66.7% ortho | c     | 1   |            | 7.726 05                 | 135.461  | 278.550 |
|                                                                      | liq   | 1   |            | 6.128 25                 | 83.5251  | 275.216 |
| <sup>2</sup> H <sub>2</sub> equilibrium,<br>97.8% ortho              | c     | 1   |            | 7.751 10                 | 135.58   | 278.50  |
|                                                                      | liq   | 1   |            | 6.044 68                 | 79.5888  | 274.680 |
| <sup>3</sup> H <sub>2</sub> (T <sub>2</sub> ) normal, 25%<br>para    | c     | 1   |            | 6.184 03                 | 76.7445  | 271.850 |
|                                                                      | liq   | 1   |            | 6.089 21                 | 81.8971  | 273.650 |
| <sup>1</sup> HBr                                                     | c     | 1   |            | 7.667 61                 | 878.57   | 253.2   |
|                                                                      | liq   | 1   |            | 6.287 53                 | 540.82   | 225.44  |
| <sup>2</sup> HBr (DBr)                                               | c     | 1   |            | 7.500 93                 | 820.68   | 247.3   |
|                                                                      | liq   | 1   |            | 6.162 38                 | 505.68   | 220.6   |
| <sup>1</sup> HCl                                                     | c     | 1   |            | 8.134 73                 | 941.57   | 268.06  |
|                                                                      | liq   | 1   |            | 7.170 00                 | 745.80   | 258.88  |
| <sup>2</sup> HCl (DCl)                                               | c     | 1   |            | 7.850 47                 | 843.32   | 258.32  |
|                                                                      | liq   | 1   |            | 6.935 96                 | 668.20   | 249.50  |
| HCN                                                                  | liq   | 1   | − 16 to 46 | 7.528 2                  | 1329.5   | 260.4   |
| <sup>1</sup> HF                                                      | liq   | 1   |            | 7.680 98                 | 1475.60  | 287.88  |
| <sup>2</sup> HF (DF)                                                 | liq   | 1   |            | 7.217 04                 | 1268.37  | 273.87  |
| <sup>1</sup> HI                                                      | c     | 1   |            | 7.315 6                  | 894.32   | 239.6   |
|                                                                      | liq   | 1   |            | 5.608 9                  | 416.04   | 188.1   |
| <sup>2</sup> HI (DI)                                                 | c     | 1   |            | 7.314 9                  | 889.52   | 238.8   |
|                                                                      | liq   | 1   |            | 5.601 8                  | 413.98   | 187.8   |
| HN <sub>3</sub>                                                      | liq   | 1   |            | 6.857                    | 1 066    | 232     |
| HNO <sub>3</sub>                                                     | liq   | 1   |            | 7.511 9                  | 1 406    | 221.0   |
| <sup>1</sup> H <sub>2</sub> O                                        |       |     |            | [See Tables 5.4 and 5.6] |          |         |
| <sup>2</sup> H <sub>2</sub> O (D <sub>2</sub> O)                     |       |     |            | [See Table 5.7]          |          |         |
| H <sub>2</sub> <sup>18</sup> O                                       |       | 1   | 0–60       | 8.133 2                  | 1 762.39 | 235.660 |
|                                                                      |       | 1   | 60–120     | 7.972 08                 | 1 668.84 | 227.700 |
| H <sub>2</sub> O <sub>2</sub>                                        | liq   | 1   |            | 7.969 17                 | 1 886.76 | 220.6   |
| HPO <sub>2</sub> F                                                   | liq   | 1   |            | 6.735 3                  | 1 342.9  | 232.0   |
| H <sub>2</sub> S                                                     | c     | 1   |            | 7.614 18                 | 885.319  | 250.25  |
|                                                                      | liq   | 1   |            | 6.993 92                 | 768.130  | 249.09  |
| H <sub>2</sub> S <sub>2</sub>                                        | liq   | 1   |            | 6.974                    | 1 232    | 225     |
| H <sub>2</sub> S <sub>3</sub>                                        | liq   | 1   |            | 6.807                    | 1 488    | 209     |
| H <sub>2</sub> S <sub>4</sub>                                        | liq   | 1   |            | 6.945                    | 1 772    | 196     |
| H <sub>2</sub> S <sub>5</sub>                                        | liq   | 1   |            | 7.320                    | 2 104    | 189     |
| HSO <sub>3</sub> Cl                                                  | liq   | 1   |            | 7.049                    | 1 480    | 201     |
| HSO <sub>3</sub> F                                                   | liq   | 1   |            | 7.399 5                  | 1 521    | 174.0   |
| H <sub>2</sub> Se                                                    | c     | 1   |            | 7.635 4                  | 927.6    | 240.0   |
|                                                                      | liq   | 1   |            | 6.966 0                  | 787.67   | 235.0   |
| H <sub>2</sub> Te                                                    | liq   | 1   |            | 7.000                    | 935      | 229     |
| <b>Iodine</b>                                                        |       |     |            |                          |          |         |
| I <sub>2</sub>                                                       | c     | 1   |            | 9.810 9                  | 2 901.0  | 256.00  |
|                                                                      | liq   | 1   |            | 7.018 1                  | 1 610.9  | 205.0   |
| ICl                                                                  | liq   | 1   |            | 7.702 1                  | 1 517.9  | 217.0   |
| IF <sub>5</sub>                                                      | c     | 1   |            | 10.964                   | 2 538    | 245     |
|                                                                      | liq   | 1   |            | 7.464 8                  | 1 460    | 216.0   |
| IF <sub>7</sub>                                                      | c     | 1   |            | 7.998                    | 1 340    | 256     |

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                       | State | Eq. | Range, °C       | A        | B        | C         |
|---------------------------------|-------|-----|-----------------|----------|----------|-----------|
| <b>Iridium</b>                  |       |     |                 |          |          |           |
| IrF <sub>6</sub>                | c     | 2   | 0.4–44          | 8.618    | 1 868    |           |
|                                 | liq   | 2   | 44–54           | 7.952    | 1 657    |           |
| <b>Iron</b>                     |       |     |                 |          |          |           |
| FeCl <sub>2</sub>               | liq   | 2   | 708–834         | 9.794    | 7 455    |           |
|                                 | liq   | 2   | 700–930         | 8.33     | 7 061    |           |
| FeCl <sub>3</sub>               | c     | 2   | 160–304         | 15.11    | 7 142    |           |
| FeI <sub>2</sub>                |       | 2   | 517–577         | 13.183   | 10 778   |           |
|                                 |       | 2   | 601–686         | 9.674    | 7 716    |           |
| <b>Krypton</b>                  |       |     |                 |          |          |           |
| Kr                              | c     | 1   |                 | 7.539 55 | 539.48   | 269.8     |
|                                 | liq   | 1   |                 | 6.630 70 | 416.38   | 264.45    |
| <b>Lead</b>                     |       |     |                 |          |          |           |
| Pb                              |       | 2   | 525–1325        | 7.827    | 9 845.4  |           |
| PbBr <sub>2</sub>               |       | 2   | 735–918         | 8.064    | 6 163.1  |           |
| PbCl <sub>2</sub>               |       | 2   | 500–950         | 8.961    | 7 411.4  |           |
| PbF <sub>2</sub>                |       | 2   | 1078–1289       | 8.391    | 8 623.2  |           |
| <b>Lithium</b>                  |       |     |                 |          |          |           |
| LiBr                            |       | 2   | 1010–1265       | 8.068    | 7 975.5  |           |
| LiCl                            |       | 2   | 1045–1325       | 7.939    | 8 142.7  |           |
| LiF                             |       | 2   | 1398–1666       | 8.753    | 11 407   |           |
| LiH                             |       | 2   | 500–650         | 11.227   | 9 600    |           |
|                                 |       | 2   | 700–800         | 9.926    | 8 204    |           |
| LiI                             |       | 2   | 940–1140        | 8.011    | 7 500    |           |
| <b>Magnesium</b>                |       |     |                 |          |          |           |
| Mg                              |       | 2   | 900–1070        | 12.993   | 13 579.8 |           |
| MgH <sub>2</sub>                |       | 2   | 337–415         | 9.78     | 3 857    |           |
| <b>Mercury</b>                  |       |     |                 |          |          |           |
| Hg                              |       |     | [See Table 5.3] |          |          |           |
| HgBr <sub>2</sub>               |       | 2   | 130–270         | 10.094   | 4 168.0  |           |
| HgCl <sub>2</sub>               |       | 2   | 130–270         | 10.094   | 4 118.34 |           |
|                                 |       | 2   | 275–309         | 8.409    | 3 187.1  |           |
| Hg <sub>2</sub> Cl <sub>2</sub> |       | 1   |                 | 8.521 51 | 3 110.96 | 168.0     |
| HgI <sub>2</sub>                |       | 2   | 266–360         | 8.115    | 3 278.5  |           |
| <b>Neon</b>                     |       |     |                 |          |          |           |
| Ne                              | c     | 1   |                 | 7.065 16 | 110.61   | 272.00    |
|                                 | liq   | 1   |                 | 6.084 44 | 78.380   | 270.550   |
| <b>Neptunium</b>                |       |     |                 |          |          |           |
| NpF <sub>6</sub>                | liq   | 3   | 55.1–76.8       | 0.010 23 | 1 191.1  | – 2.582 5 |
| <b>Nickel</b>                   |       |     |                 |          |          |           |
| Ni(CO) <sub>4</sub>             |       | 2   | 2–40            | 7.780    | 1 556.5  |           |
| <b>Niobium</b>                  |       |     |                 |          |          |           |
| NbBr <sub>5</sub>               | liq   | 2   |                 | 8.92     | 3 850    |           |
| NbCl <sub>5</sub>               | liq   | 2   | 210–254         | 8.37     | 2 827    |           |
| NbF <sub>5</sub>                | liq   | 2   |                 | 8.439    | 2 824    |           |
| <b>Nitrogen</b>                 |       |     |                 |          |          |           |
| N <sub>2</sub> natural          | c     | 1   |                 | 7.345 12 | 322.222  | 269.980   |
|                                 | liq   | 1   |                 | 6.494 57 | 255.680  | 266.550   |
| <sup>15</sup> N <sub>2</sub>    | c     | 1   |                 | 7.363 96 | 323.17   | 269.88    |
|                                 | liq   | 1   |                 | 6.494 14 | 255.535  | 266.451   |
| NCl <sub>3</sub>                |       | 1   |                 | 6.956    | 1 190    | 221       |
| NF <sub>3</sub>                 | liq   | 1   |                 | 6.779 66 | 501.913  | 257.79    |
| NH <sub>3</sub>                 |       |     | [See Table 5.5] |          |          |           |

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                                 | State  | Eq. | Range, °C        | A         | B         | C       |
|-------------------------------------------|--------|-----|------------------|-----------|-----------|---------|
| <b>Nitrogen</b> ( <i>continued</i> )      |        |     |                  |           |           |         |
| N <sub>2</sub> H <sub>4</sub>             | liq    | 1   |                  | 7.801 9   | 1 679.07  | 227.7   |
| NO natural                                | c      | 1   |                  | 9.628 26  | 758.736   | 266.00  |
|                                           | liq    | 1   |                  | 8.743 00  | 682.938   | 268.27  |
| N <sub>2</sub> O                          | c      | 1   |                  | 9.437 00  | 1 174.020 | 268.22  |
|                                           | liq    | 1   |                  | 7.003 94  | 654.260   | 247.16  |
| N <sub>2</sub> O <sub>4</sub> equilibrium | c      | 1   |                  | 10.736 31 | 2 075.53  | 252.80  |
| mixture                                   | liq    | 1   |                  | 8.917 12  | 1 798.54  | 276.80  |
| N <sub>2</sub> O <sub>5</sub>             | c      | 1   |                  | 11.644 5  | 2 510     | 253.0   |
| NOCl                                      | c      | 1   |                  | 8.540 8   | 1 397.3   | 261.0   |
|                                           | liq    | 1   |                  | 7.361 54  | 1 094.73  | 249.70  |
| N <sub>2</sub> O <sub>3</sub>             |        | 2   | − 25 to 0        | 10.30     | 2 057.9   |         |
| NOF                                       | liq    | 1   |                  | 6.443 5   | 556.13    | 216.0   |
| NO <sub>2</sub> Cl                        | liq    | 1   |                  | 5.372 3   | 395.40    | 174.0   |
| NO <sub>2</sub> F                         | liq    | 1   |                  | 6.833 4   | 654.55    | 238.0   |
| <b>Osmium</b>                             |        |     |                  |           |           |         |
| OsF <sub>5</sub>                          |        | 2   | 75–180           | 9.75      | 3 429     |         |
| OsF <sub>6</sub>                          |        | 2   | 34–48            | 7.470     | 1 473     |         |
| OsF <sub>8</sub>                          |        | 2   | 38–47            | 7.650     | 1 525     |         |
| OsO <sub>4</sub>                          |        | 2   | − 38 to 40       | 10.710 0  | 2 951.00  |         |
| OsO <sub>3</sub> F <sub>2</sub>           |        | 2   | 59–105           | 7.994     | 1 911     |         |
| <b>Oxygen</b>                             |        |     |                  |           |           |         |
| O <sub>2</sub>                            | liq    | 1   |                  | 6.691 44  | 319.013   | 266.697 |
| O <sub>3</sub>                            | liq    | 1   |                  | 6.837     | 552.5     | 251.0   |
| OF <sub>2</sub>                           | liq    | 1   |                  | 7.236 19  | 545.05    | 269.91  |
| O <sub>2</sub> F <sub>2</sub>             | liq    | 1   |                  | 6.779 02  | 756.39    | 250.16  |
| O <sub>3</sub> F <sub>2</sub>             |        | 2   | 79–114           | 6.134 3   | 675.57    |         |
| <b>Palladium</b>                          |        |     |                  |           |           |         |
| PdCl <sub>2</sub>                         |        | 2   | 680–857          | 6.32      | 5 032     |         |
| <b>Phosphorus</b>                         |        |     |                  |           |           |         |
| P red, V                                  | subl c | 1   |                  | 11.060    | 5 323     | 220     |
| white                                     | subl c | 1   |                  | 6.936 9   | 1 907.6   | 190.0   |
| P <sub>4</sub> black, o-rh                |        | 1   |                  | 12.405    | 6 671     | 247     |
| PBr <sub>3</sub>                          | liq    | 1   | − 40 to 173      | 6.915 5   | 1 590.5   | 221.0   |
| PBr <sub>5</sub>                          | liq    | 1   | to 104           | 6.948     | 1 320     | 214     |
| PBrF <sub>2</sub>                         | liq    | 1   | − 133 to − 16    | 6.904 2   | 885.12    | 236.0   |
| PBr <sub>2</sub> F                        | liq    | 1   | − 115 to 78      | 6.858 0   | 1 210.3   | 226.0   |
| PCl <sub>3</sub>                          | liq    | 1   | − 92 to 76       | 6.826 7   | 1 196     | 227.0   |
| PCl <sub>5</sub>                          | c      | 1   | to 160           | 10.206 8  | 2 903.1   | 237.0   |
|                                           | liq    | 1   |                  | 7.033     | 1 490     | 200.0   |
| PClF <sub>2</sub>                         | liq    | 1   | − 165 to − 47    | 6.639 6   | 780.88    | 255.0   |
| PCL <sub>2</sub> F                        | liq    | 1   | − 144 to 14      | 6.796 56  | 982.332   | 237.00  |
| P(OCN) <sub>3</sub>                       | liq    | 2   | − 2 to 169       | 8.745 5   | 2 595     |         |
| PF <sub>3</sub>                           | liq    | 1   | − 152 to − 101   | 6.860 4   | 620.22    | 257.0   |
| PF <sub>5</sub>                           | liq    | 1   | − 93.8 to − 84.5 | 6.914 4   | 647.21    | 245.0   |
| PH <sub>3</sub>                           | c      | 1   |                  | 7.482 35  | 794.496   | 265.20  |
|                                           | liq    | 1   |                  | 6.715 59  | 645.512   | 256.066 |
| P <sub>2</sub> H <sub>4</sub>             | liq    | 1   |                  | 6.862 8   | 1 137     | 227.0   |
| P <sub>4</sub> O <sub>6</sub>             | liq    | 1   | 24–175           | 6.716 37  | 1 412.8   | 193.0   |
| P <sub>4</sub> O <sub>10</sub>            | c III  | 1   |                  | 9.707 0   | 3 822     | 201.0   |
|                                           | c I    | 1   |                  | 10.843 2  | 6 424     | 213     |
|                                           | liq    | 1   |                  | 6.935 2   | 3 069     | 152     |
| POBr <sub>3</sub>                         | liq    | 1   | 51–192           | 7.007 8   | 1 609.2   | 198.0   |



TABLE 5.8 Vapor Pressures of Various Inorganic Compounds (Continued)

| Substance                      | State | Eq. | Range, °C      | A          | B        | C         |
|--------------------------------|-------|-----|----------------|------------|----------|-----------|
| <b>Phosphorus</b> (continued)  |       |     |                |            |          |           |
| POBrCl <sub>2</sub>            | liq   | 1   | 31–165         | 6.924      | 1 411    | 213       |
| POBrClF                        | liq   | 1   |                | 6.914      | 1 214    | 222       |
| POBrF <sub>2</sub>             | liq   | 1   | – 85 to 32     | 7.101 9    | 1 118.9  | 233.0     |
| POBr <sub>2</sub> F            | liq   | 1   | – 117 to 110   | 6.721 2    | 1 328.9  | 236.0     |
| POCl <sub>3</sub>              | liq   | 1   | 1.2–105        | 6.865 8    | 1 297.2  | 220.0     |
| POClF <sub>2</sub>             | liq   | 1   | – 96 to 3      | 6.926 6    | 946.96   | 231.0     |
| POCl <sub>2</sub> F            | liq   | 1   | – 80 to 53     | 7.084 65   | 1 201.86 | 233.00    |
| POF <sub>3</sub>               | c     | 1   |                | 10.930 5   | 1 783    | 261.0     |
|                                | liq   | 1   |                | 7.115 5    | 810.1    | 231.0     |
| PO(OCN) <sub>3</sub>           |       | 2   | 5–193          | 9.168 2    | 2 931    |           |
| PO(SCN) <sub>3</sub>           |       | 2   | 14–300         | 8.533 0    | 3 240    |           |
| P <sub>4</sub> S <sub>10</sub> |       | 2   |                | 9.17       | 4 940    |           |
| PSBr <sub>3</sub>              | c     | 2   |                | 10.105     | 3 196.2  |           |
|                                | liq   | 2   |                | 8.338 3    | 2 641.9  |           |
| PS(OCN) <sub>3</sub>           |       | 2   |                | 10.032     | 3 492    |           |
| <b>Platinum</b>                |       |     |                |            |          |           |
| Pt                             |       | 2   | 1425–1765      | 7.786      | 25 384   |           |
| PtF <sub>6</sub>               | liq   | 1   | 61.3–81.7      | 89.15      | 5 686    | 27.49     |
| <b>Polonium</b>                |       |     |                |            |          |           |
| Po                             | liq   | 1   |                | 7.041 4    | 5 017.6  | 241.0     |
| PoCl <sub>4</sub>              | liq   | 1   |                | 7.554      | 2 360    | 115       |
| <b>Potassium</b>               |       |     |                |            |          |           |
| K                              |       | 2   | 260–760        | 7.183      | 4 434.33 |           |
| KBr                            |       | 2   | 1095–1375      | 7.936      | 8 555.3  |           |
| KCl                            |       | 2   | 1116–1418      | 8.130      | 8 863.4  |           |
| KF                             |       | 2   | 1278–1500      | 9.000      | 10 838   |           |
| KOH                            |       | 2   | 1170–1327      | 7.330      | 7 103.3  |           |
| KI                             |       | 2   | 1063–1333      | 7.949      | 8 132.2  |           |
| <b>Protactinium</b>            | liq   | 2   |                | 17.27      | 7 377    |           |
| <b>Radon</b>                   |       |     |                |            |          |           |
| Rn                             | c     | 1   |                | 7.495 5    | 884.41   | 255.0     |
|                                | liq   | 1   |                | 6.701 5    | 718.25   | 250.0     |
| <b>Rhenium</b>                 |       |     |                |            |          |           |
| ReF <sub>5</sub>               | c     | 2   |                | 9.024      | 3 037    |           |
| ReF <sub>6</sub>               | c     | 3   | – 3.45 to 18.5 | 9.123 0    | 1 765.4  | 0.1790    |
|                                | liq   | 3   | 18.5–48        | 18.208 1   | 1 956.7  | 3.599     |
| ReF <sub>7</sub>               | c     | 3   | – 14.5 to 48.3 | 13.043 2   | 2 205.8  | 1.470 3   |
|                                | liq   | 3   | 48.3–74.6      | – 21.583 5 | 244.28   | – 9.908 3 |
| ReO <sub>2</sub>               | c     | 2   | 650–785        | 11.65      | 14 437   |           |
|                                | liq   | 2   | 480–660        | 5.345      | 4 742    |           |
| ReO <sub>3</sub>               | c     | 2   | 325–420        | 15.16      | 10 882   |           |
|                                | liq   | 2   | 300–480        | 7.745      | 4 966    |           |
| Re <sub>2</sub> O <sub>7</sub> | liq   | 2   | 230–360        | 8.98       | 3 868    |           |
| ReOF <sub>4</sub>              | liq   | 2   | 108–172        | 10.09      | 3 206    |           |
| ReOF <sub>5</sub>              | liq   | 2   | 41–73          | 7.727      | 1 679    |           |
| ReS <sub>2</sub>               | c     | 2   | 500–700        | 3.214      | 4 976    |           |
| Re <sub>2</sub> S <sub>7</sub> | c     | 2   | 260–410        | 8.86       | 4 800    |           |
| <b>Rubidium</b>                |       |     |                |            |          |           |
| Rb                             |       | 2   | 250–370        | 6.976      | 3 969.5  |           |
| RbCl                           |       | 2   | 1142–1395      | 9.111      | 10 373   |           |
| RbF                            |       | 2   | 1142–1400      | 8.570      | 9 568.4  |           |

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                                     | State | Eq. | Range, °C       | A        | B        | C       |
|-----------------------------------------------|-------|-----|-----------------|----------|----------|---------|
| <b>Ruthenium</b>                              |       |     |                 |          |          |         |
| RuOF <sub>4</sub>                             |       | 2   | 120–160         | 8.60     | 2 616    |         |
| <b>Selenium</b>                               |       |     |                 |          |          |         |
| Se                                            | liq   | 1   |                 | 7.631 6  | 4 213.0  | 202.0   |
| SeCl <sub>4</sub>                             | c     | 1   |                 | 10.250 9 | 3 068.8  | 225.0   |
| SeF <sub>4</sub>                              | liq   | 1   |                 | 7.888 7  | 1 603.0  | 215.0   |
| SeF <sub>6</sub>                              | c     | 1   |                 | 8.385 4  | 1 121.4  | 250.0   |
| SeO <sub>2</sub>                              |       | 1   |                 | 6.577 81 | 1 879.81 | 179.0   |
| SeOCl <sub>2</sub>                            | liq   | 1   |                 | 6.257 3  | 970.87   | 112.0   |
| SeOF <sub>2</sub>                             | liq   | 1   |                 | 7.420    | 1 380    | 178     |
| <b>Silicon</b>                                |       |     |                 |          |          |         |
| SiCl <sub>4</sub>                             | liq   | 1   | 0–53            | 6.857 26 | 1 138.92 | 228.88  |
| SiH <sub>4</sub>                              |       | 2   | – 160 to – 112  | 6.881    | 645.9    |         |
| Si <sub>2</sub> H <sub>6</sub>                |       | 2   | – 115 to – 14.6 | 7.258    | 1 133.4  |         |
| Si <sub>3</sub> H <sub>8</sub>                |       | 2   | – 70 to 52      | 7.676    | 1 559.1  |         |
| <b>Silver</b>                                 |       |     |                 |          |          |         |
| AgCl                                          |       | 2   | 1255–1442       | 8.179    | 9 688.7  |         |
| <b>Sodium</b>                                 |       |     |                 |          |          |         |
| Na                                            |       | 2   | 180–883         | 7.553    | 5 395.4  |         |
| NaCl                                          |       | 2   | 976–1155        | 8.329 7  | 9 417.07 |         |
| NaCl                                          |       | 2   | 1156–1430       | 8.548    | 9 704.3  |         |
| NaCN                                          |       | 2   | 800–1360        | 7.472    | 8 122.81 |         |
| NaF                                           |       | 2   | 1562–1701       | 8.640    | 11 396.6 |         |
| NaI                                           |       | 2   | 1063–1307       | 8.371    | 8 623.2  |         |
| NaOH                                          |       | 2   | 1010–1402       | 7.030    | 6 894    |         |
| <b>Strontium</b>                              |       |     |                 |          |          |         |
| Sr                                            |       | 2   | 940–1140        | 16.056   | 18 802.8 |         |
| <b>Sulfur</b>                                 |       |     |                 |          |          |         |
| S equilibrium                                 | liq   | 1   |                 | 6.843 59 | 2 500.12 | 186.30  |
| S <sub>2</sub> Br <sub>2</sub>                | liq   | 1   |                 | 7.177    | 1 660    | 185     |
| SCL <sub>2</sub>                              | liq   | 1   |                 | 8.454    | 1 594    | 227     |
| S <sub>2</sub> Cl <sub>2</sub>                | liq   | 1   |                 | 6.783 6  | 1 341    | 206.0   |
| S <sub>2</sub> F <sub>2</sub>                 | liq   | 1   |                 | 6.684    | 628      | 256     |
| SF <sub>4</sub>                               | liq   | 1   |                 | 6.839 5  | 823.4    | 248.0   |
| SF <sub>6</sub>                               | c     | 1   |                 | 8.416 0  | 1 096.5  | 262.0   |
| S <sub>2</sub> F <sub>10</sub>                | liq   | 1   |                 | 7.067 6  | 1 100.6  | 234.0   |
| SO <sub>2</sub>                               | c     | 1   |                 | 9.754 3  | 1 553.8  | 225.0   |
|                                               | liq   | 1   |                 | 7.282 28 | 999.900  | 237.190 |
| SO <sub>3</sub> “icelike”                     | c III | 1   |                 | 10.565 7 | 2 273.8  | 255.0   |
| “woollike”                                    | c II  | 1   |                 | 11.590 1 | 2 665.6  | 264.0   |
|                                               | c I   | 1   |                 | 14.255 9 | 3 692.1  | 273.0   |
|                                               | liq   | 1   |                 | 9.050 85 | 1 735.31 | 236.50  |
| SOBr <sub>2</sub>                             | liq   | 1   |                 | 7.056    | 1 445    | 206     |
| SOCl <sub>2</sub>                             | liq   | 1   |                 | 7.287 45 | 1 446.7  | 252.7   |
| SOCIF                                         | liq   | 1   |                 | 7.173 1  | 1 100.1  | 244.00  |
| SOF <sub>2</sub>                              | liq   | 1   |                 | 6.959 06 | 775.48   | 234.00  |
| SOF <sub>4</sub>                              | liq   | 1   |                 | 7.071 8  | 840.3    | 249.0   |
| S <sub>2</sub> O <sub>2</sub> F <sub>10</sub> | liq   | 1   |                 | 6.874    | 1 110    | 229     |
| S <sub>2</sub> O <sub>5</sub> Cl <sub>2</sub> | liq   | 1   |                 | 7.019    | 1 460    | 202     |
| S <sub>2</sub> O <sub>5</sub> ClF             | liq   | 1   |                 | 7.015 6  | 1 257.4  | 204.0   |
| S <sub>2</sub> O <sub>5</sub> F <sub>2</sub>  | liq   | 1   |                 | 6.881    | 1 120    | 229     |
| S <sub>2</sub> O <sub>5</sub> F <sub>4</sub>  | liq   | 1   |                 | 6.885    | 1 140    | 227     |

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                                        | State  | Eq. | Range, °C     | A        | B         | C       |
|--------------------------------------------------|--------|-----|---------------|----------|-----------|---------|
| <b>Sulfur</b> ( <i>continued</i> )               |        |     |               |          |           |         |
| SO <sub>2</sub> BrF                              | liq    | 1   |               | 7.142 8  | 1 155     | 231.0   |
| SO <sub>2</sub> Cl <sub>2</sub>                  | liq    | 1   |               | 7.001 7  | 1 209     | 224.0   |
| SO <sub>2</sub> ClF                              | liq    | 1   |               | 6.521 5  | 793.73    | 210.70  |
| SO <sub>2</sub> F <sub>2</sub>                   | liq    | 1   |               | 6.907 0  | 784.3     | 250     |
| <b>Tantalum</b>                                  |        |     |               |          |           |         |
| TaBr <sub>5</sub>                                | liq    | 2   |               | 8.11     | 3 260     |         |
| TaCl <sub>5</sub>                                | liq    | 2   | 220–240       | 8.68     | 2 970     |         |
| TaF <sub>5</sub>                                 | liq    | 2   |               | 8.524    | 2 834     |         |
| TaI <sub>5</sub>                                 | liq    | 2   |               | 7.67     | 3 950     |         |
| <b>Technetium</b>                                |        |     |               |          |           |         |
| TcF <sub>6</sub>                                 | liq    | 3   | 37.4–51.7     | 24.808 7 | 2 405     | 5.803 6 |
| TcO <sub>3</sub> F                               | liq    | 2   | 18.3–51.8     | 8.417    | 2 065     |         |
| Tc <sub>2</sub> O <sub>7</sub>                   | c      | 2   |               | 18.279   | 7 205     |         |
|                                                  | liq    | 2   |               | 8.999    | 3 571     |         |
| <b>Tellurium</b>                                 |        |     |               |          |           |         |
| Te                                               | liq    | 1   |               | 7.301 0  | 5 370.6   | 221     |
| TeCl <sub>4</sub>                                | liq    | 1   |               | 7.558 6  | 2 355     | 115     |
| TeF <sub>6</sub>                                 | liq    | 1   |               | 6.748 8  | 807.0     | 247.0   |
| Te <sub>2</sub> F <sub>10</sub>                  | liq    | 1   |               | 6.901 8  | 1 150     | 227.0   |
| TeO <sub>2</sub>                                 |        | 2   | 450–733       | 12.328 4 | 13 222    |         |
| <b>Thallium</b>                                  |        |     |               |          |           |         |
| Tl                                               |        | 2   | 950–1200      | 6.1240   | 6 268     |         |
| TlF                                              |        | 2   | 282–298       | 12.52    | 5 484     |         |
| <b>Thorium</b>                                   |        |     |               |          |           |         |
| ThF <sub>4</sub>                                 | liq    | 2   |               | 10.821   | 15 270    |         |
| ThH <sub>2</sub>                                 |        | 2   | up to 883     | 9.50     | 7 650     |         |
| <b>Tin</b>                                       |        |     |               |          |           |         |
| SnCl <sub>4</sub>                                |        | 2   | – 52 to – 38  | 9.824    | 2 441.23  |         |
| SnH <sub>4</sub>                                 |        | 2   | – 148 to – 49 | 7.400    | 999.68    |         |
| <b>Titanium</b>                                  |        |     |               |          |           |         |
| TiCl <sub>2</sub>                                | subl c | 2   |               | 9.30     | 8 500     |         |
| TiCl <sub>3</sub>                                | subl c | 2   | 455–550       | 10.401   | 8 296     |         |
| TiCl <sub>4</sub>                                | liq    | 2   | – 23 to 136   | 7.683    | 1 964     |         |
| TiI <sub>4</sub>                                 | liq    | 2   | 160–360       | 7.577    | 3 054     |         |
| <b>Tungsten</b>                                  |        |     |               |          |           |         |
| W                                                |        | 2   | 2230–2770     | 9.920    | 46 850    |         |
| <b>Uranium</b>                                   |        |     |               |          |           |         |
| UF <sub>6</sub>                                  | liq    | 1   | 64–116        | 6.994 64 | 1 126.288 | 221.963 |
|                                                  | liq    | 1   | 116–230       | 7.690 69 | 1 683.165 | 302.148 |
| UH <sub>3</sub> dissociation                     |        | 2   | 200–430       | 9.39     | 4 590     |         |
| U <sup>2</sup> H <sub>3</sub> (UD <sub>3</sub> ) |        | 2   |               | 9.43     | 4 500     |         |
| U <sup>3</sup> H <sub>3</sub> (UT <sub>3</sub> ) |        | 2   |               | 9.46     | 4 471     |         |
| <b>Vanadium</b>                                  |        |     |               |          |           |         |
| VBr <sub>2</sub>                                 | c      | 2   | 541–716       | 9.08     | 10 460    |         |
|                                                  | subl c | 2   | 800–905       | 5.9      | 9 830     |         |
| VBr <sub>3</sub>                                 |        | 2   | 314–427       | 11.12    | 7 470     |         |
| VCl <sub>2</sub>                                 | subl c | 2   | 910–1100      | 5.725    | 9 721     |         |
| VCl <sub>3</sub>                                 |        | 2   | 352–567       | 11.20    | 9 777     |         |
| VCl <sub>4</sub>                                 | liq    | 2   | 30–153        | 7.62     | 2 020     |         |
| VF <sub>3</sub>                                  | subl c | 2   | 650–920       | 12.357   | 15 603    |         |
| VF <sub>5</sub>                                  | subl c | 2   | – 20 to 19.5  | 8.168    | 2 608     |         |
|                                                  | liq    | 2   | 19.5–45.5     | 7.549    | 2 423     |         |

**TABLE 5.8** Vapor Pressures of Various Inorganic Compounds (*Continued*)

| Substance                            | State  | Eq. | Range, °C | A         | B        | C       |
|--------------------------------------|--------|-----|-----------|-----------|----------|---------|
| <b>Vanadium</b> ( <i>continued</i> ) |        |     |           |           |          |         |
| VI <sub>2</sub>                      | subl c | 2   | 850–1016  | 2.56      | 5 600    |         |
| VOCl <sub>3</sub>                    | liq    | 2   | 15.4–125  | 7.69      | 1 920    |         |
| <b>Xenon</b>                         |        |     |           |           |          |         |
| Xe                                   | c      | 1   |           | 7.484 5   | 714.896  | 264.0   |
|                                      | liq    | 1   |           | 6.642 89  | 566.282  | 258.660 |
| XeF <sub>2</sub>                     | subl c | 1   |           | 10.019 47 | 2 683.96 | 261.68  |
| XeF <sub>4</sub>                     | subl c | 1   |           | 10.913 87 | 3 095.06 | 269.56  |
| <b>Zinc</b>                          |        |     |           |           |          |         |
| Zn                                   | c      | 2   | 250–419   | 9.200     | 6 946.6  |         |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds

| Substance                       | Eq. | Range, °C   | A         | B         | C        |
|---------------------------------|-----|-------------|-----------|-----------|----------|
| Acenaphthene                    | 1   | 147–187     | 7.728 19  | 2 534.234 | 245.576  |
|                                 | 2   | 147–288     | 8.033     | 2 834.99  |          |
| Acetaldehyde                    | 1   | liq         | 8.005 52  | 1 600.017 | 291.809  |
| Acetic acid                     | 1   | liq         | 7.387 82  | 1 533.313 | 222.309  |
| Acetic anhydride                | 1   | liq         | 7.149 48  | 1 444.718 | 199.817  |
| Acetone                         | 1   | liq         | 7.117 14  | 1 210.595 | 229.664  |
| Acetonitrile                    | 1   | liq         | 7.119 88  | 1 314.4   | 230      |
| Acetophenone                    | 2   | 30–100      | 9.135 2   | 2 878.8   |          |
| Acetyl bromide                  | 1   | liq         | 5.197 02  | 545.784   | 150.396  |
| Acetyl chloride                 | 1   | liq         | 6.948 87  | 1 115.954 | 223.554  |
| Acetylene                       | 1   | –130 to –83 | 9.140 2   | 1 232.6   | 280.9    |
|                                 | 1   | –82 to –72  | 7.099 9   | 711.0     | 253.4    |
| Acetyl iodide                   | 1   | liq         | 4.181 44  | 355.452   | 108.160  |
| Acrylic acid                    | 1   | 20–70       | 8.538 67  | 2305.843  | 266.547  |
| Acrylonitrile                   | 1   | –20 to 140  | 7.038 55  | 1 232.53  | 222.47   |
| Allyl isothiocyanate            | 1   | 10–50       | 5.126 58  | 791.434   | 154.019  |
| <i>m</i> -Aminobenzotrifluoride | 1   | 0–96        | 7.651 86  | 1 940.6   | 218.0    |
|                                 |     | 96–300      | 7.170 30  | 1 650.21  | 193.58   |
| <i>p</i> -Aminophenol           | 1   | 130–185     | –3.357 50 | 699.157   | –331.343 |
| Aniline                         | 1   | 102–185     | 7.320 10  | 1 731.515 | 206.049  |
| Anthracene                      | 2   | 100–160     | 8.91      | 3 761     |          |
|                                 | 1   | 176–380     | 7.674 01  | 2 819.63  | 247.02   |
| 9,10-Anthracenedione            | 2   | 224–286     | 12.305    | 5 747.9   |          |
|                                 | 2   | 285–370     | 8.002     | 3 341.94  |          |
| Benzene                         | 1   | –12 to 3    | 9.106 4   | 1 885.9   | 244.2    |
|                                 | 1   | 8–103       | 6.905 65  | 1 211.033 | 220.790  |
| Benzenethiol                    | 1   | 52–198      | 6.990 19  | 1 529.454 | 203.048  |
| Benzoic acid                    | 2   | 60–110      | 9.033     | 3 333.3   |          |
| Benzonitrile                    | 1   | liq         | 6.746 31  | 1 436.72  | 181.0    |
| Benzophenone                    | 1   | 48–202      | 7.349 66  | 2 331.4   | 195.0    |
|                                 | 1   | 200–306     | 7.162 94  | 2 051.855 | 173.074  |
| Benzotrifluoride                | 1   | –20 to 180  | 7.007 08  | 1 331.30  | 220.58   |
| Benzoyl chloride                | 2   | 140–200     | 7.924 5   | 2 372.1   |          |
| Benzyl acetate                  | 1   | 46–156      | 8.457 05  | 2 623.206 | 259.067  |
| Benzyl alcohol                  | 1   | 122–205     | 7.198 17  | 1 632.593 | 172.790  |

TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                                     | Eq. | Range, °C  | A        | B         | C       |
|-----------------------------------------------|-----|------------|----------|-----------|---------|
| Biphenyl                                      | 1   | 69–271     | 7.245 41 | 1 998.725 | 202.733 |
| 2-(2-Biphenyloxy)ethanol                      | 1   | 240–300    | 8.005 87 | 2 776.761 | 206.914 |
| Bromobenzene                                  | 1   | 56–154     | 6.860 64 | 1 438.817 | 205.441 |
| 2-Bromobenzyl cyanide                         | 1   | 85–152     | 5.044 59 | 734.821   | 59.273  |
| 1-Bromobutane                                 | 1   | –78 to 23  | 5.281 38 | 685.001   | 160.880 |
| Bromochloromethane                            | 1   | 16–68      | 6.496 06 | 942.267   | 192.587 |
| Bromochlorodifluoromethane                    | 1   | –95 to 10  | 6.839 98 | 935.632   | 240.330 |
| 2-Bromo-2-chloro-1,1,1-trifluoroethane        | 1   | –51 to 55  | 6.945 02 | 1 127.856 | 227.341 |
| Bromocyclohexane                              | 1   | 68–260     | 6.979 80 | 1 572.19  | 217.38  |
| <i>p</i> -Bromodiphenyl ether                 | 1   | 25–190     | 7.009 3  | 1 902.7   | 153.3   |
|                                               | 1   | 190–400    | 6.681 43 | 1 683.84  | 132.90  |
| Bromoethane                                   | 1   | 28–75      | 6.988 6  | 1 121.9   | 234.7   |
| Bromoethene                                   | 1   | –88 to 16  | 6.997 4  | 1 009.9   | 251.6   |
| 2-Bromoethylbenzene                           | 1   | 127–217    | 7.800    | 2 235.4   | 238.7   |
| 4-Bromoethylbenzene                           | 1   | liq        | 6.982 09 | 1 632.60  | 193     |
| 2-Bromo-2-methylpropane                       | 1   | 0–72.8     | 7.395 9  | 1 512.7   | 262.2   |
| 1-Bromonaphthalene                            | 1   | liq        | 7.003 50 | 1 927.05  | 186.0   |
| <i>o</i> -Bromostyrene                        | 1   | liq        | 6.910 38 | 1 631.2   | 195     |
| <i>p</i> -Bromostyrene                        | 1   |            | 7.228 38 | 1 743.67  | 218.0   |
| 4-Bromotoluene                                | 1   | 85–280     | 7.007 62 | 1 612.35  | 206.36  |
| 2-Bromovinylbenzene                           | 1   | 110–129    | 0.564 97 | 82.913    | –191.71 |
| 4-Bromovinylbenzene                           | 1   | 119–147    | 12.504 2 | 7 349.00  | 559.02  |
| 1,2-Butadiene                                 | 1   | –69 to –34 | 7.398 22 | 1 219.877 | 259.776 |
|                                               | 1   | –26 to 30  | 6.993 83 | 1 041.117 | 242.274 |
| 1,3-Butadiene                                 | 1   | –80 to –62 | 7.035 55 | 998.106   | 245.233 |
|                                               | 1   | –58 to 15  | 6.849 99 | 930.546   | 238.854 |
| <i>n</i> -Butane                              | 1   | –77 to 19  | 6.808 96 | 935.86    | 238.73  |
| 1-Butanethiol                                 | 1   | –2 to 123  | 6.927 54 | 1 281.018 | 218.100 |
| 2-Butanethiol                                 | 1   | –13 to 110 | 6.886 98 | 1 229.904 | 222.021 |
| 1-Butanol                                     | 1   | 15–131     | 7.476 80 | 1 362.39  | 178.77  |
| 2-Butanol                                     | 1   | 25–120     | 7.474 31 | 1 314.19  | 186.55  |
| 2-Butanone                                    | 1   | 43–88      | 7.063 56 | 1 261.34  | 221.97  |
| 1-Butene                                      | 1   | –82 to 13  | 6.792 90 | 908.80    | 238.54  |
| 2-Butene <i>cis</i>                           | 1   | –73 to 23  | 6.884 68 | 967.32    | 237.87  |
| <i>trans</i>                                  | 1   | –76 to 20  | 6.883 37 | 967.50    | 240.84  |
| Butyl acetate                                 | 1   | 60–126     | 7.127 12 | 1 430.418 | 210.745 |
| <i>n</i> -Butylamine trimethylboron           | 1   | 0–99       | 8.465 21 | 1 980.98  | 193.60  |
| <i>n</i> -Butylbenzene                        | 1   | 62–213     | 6.983 17 | 1 577.965 | 201.378 |
| <i>sec</i> -Butylbenzene                      | 1   | 87–174     | 6.942 19 | 1 533.95  | 204.39  |
| <i>t</i> -Butylbenzene                        | 1   | 84–170     | 6.922 55 | 1 505.987 | 203.490 |
| <i>n</i> -Butyl borate                        | 1   | 117–218    | 7.406 87 | 1 905.035 | 186.134 |
| <i>n</i> -Butyl- <i>t</i> -butyl ether        | 1   | 83–124     | 6.955 56 | 1 348.702 | 206.303 |
| Butyl carbitol                                | 1   | 50–153     | 7.741 14 | 2 056.904 | 195.655 |
| Butyl cellosolve                              | 1   | 93–170     | 6.956 59 | 1 399.903 | 172.154 |
| <i>sec</i> -Butyl chloroacetate               | 1   | 30–172     | 7.933 38 | 2 103.30  | 249.29  |
| <i>n</i> -Butylcyclohexane                    | 1   | 60–211     | 6.910 30 | 1 538.518 | 200.833 |
| <i>sec</i> -Butylcyclohexane                  | 1   | 91–180     | 6.890 96 | 1 530.70  | 202.373 |
| <i>t</i> -Butylcyclohexane                    | 1   | 84–173     | 6.856 80 | 1 501.724 | 206.108 |
| <i>n</i> -Butylcyclopentane                   | 1   | 41–185     | 6.899 35 | 1 457.08  | 205.99  |
| <i>n</i> -Butyl formate                       | 1   | 29–112     | 7.693 6  | 1 698.7   | 247.4   |
| <i>sec</i> -Butyl formate                     | 1   | 30–100     | 6.493    | 972.9     | 176.0   |
| <i>n</i> -Butyl- $\alpha$ -hydroxyisobutyrate | 1   | 112–185    | 8.421 7  | 2 617.32  | 287.09  |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                        | Eq. | Range, °C   | A        | B         | C      |
|----------------------------------|-----|-------------|----------|-----------|--------|
| 1- <i>n</i> -Butylnaphthalene    | 1   | 25–170      | 7.434 47 | 2 227.7   | 202.2  |
|                                  | 1   | 170–345     | 7.081 4  | 1 971.5   | 180    |
| 2- <i>n</i> -Butylnaphthalene    | 1   | 25–170      | 7.438 08 | 2 242.2   | 202.3  |
|                                  | 1   | 170–345     | 7.084 8  | 1 984.3   | 180    |
| <i>n</i> -Butyl nitrate          | 1   | 0–70        | 8.054 27 | 1 992.83  | 254.30 |
| 1-Butyl pentafluoropropionate    | 1   | 82–116      | 6.651 00 | 1 108.02  | 177.04 |
| 2- <i>sec</i> -Butylphenol       | 1   | 179–240     | 6.951 93 | 1 593.74  | 163.79 |
| 2- <i>t</i> -Butylphenol         | 1   | 135–225     | 7.217 56 | 1 822.81  | 196.23 |
| 4- <i>t</i> -Butylphenol         | 1   | 198–252     | 7.000 38 | 1 627.51  | 155.24 |
| Butyl phenyl ether               | 1   | 119–210     | 7.299 7  | 1 882.70  | 215.82 |
| <i>n</i> -Butyl propionate       | 1   | 32–93       | 9.484 89 | 2 852.58  | 296.98 |
| <i>n</i> -Butyl trifluoroacetate | 1   | 71–104      | 8.567 94 | 2 305.22  | 301.06 |
| 1-Butyl trimethylsilyl ether     | 1   | 71–124      | 7.763 00 | 1 884.68  | 261.31 |
| 1-Butyne                         | 1   | –68 to 27   | 6.981 98 | 988.75    | 233.01 |
| 2-Butyne                         | 1   | –51 to –34  | 7.037 91 | 896.91    | 199.06 |
|                                  | 1   | –31 to 47   | 7.073 38 | 1 101.71  | 235.81 |
| <i>n</i> -Butyraldehyde          | 1   | 31–74       | 6.385 44 | 913.59    | 185.48 |
| Butyric acid                     | 1   | 90–163      | 7.739 9  | 1 764.7   | 199.9  |
| Camphor                          | 2   | 0–180       | 8.799    | 2 797.39  |        |
|                                  | 1   | 178–232     | 6.106    | 1 043.6   | 116.4  |
| Capric acid                      | 1   | 153–187     | 6.255 3  | 1 106.3   | 57.96  |
| Caproic acid                     | 1   | 98–179      | 6.924 9  | 1 340.8   | 126.6  |
| Capronitrile                     | 1   | 92–164      | 7.123 1  | 1 597.2   | 212.8  |
| Caprylic acid                    | 1   | 130–206     | 7.770 64 | 1 933.05  | 159.36 |
| Carbazole                        | 1   | 253–358     | 7.086 3  | 2 179.4   | 163.5  |
| Carbitol                         | 1   | 40–151      | 7.640 81 | 1 801.31  | 183.97 |
| Chloroacetic acid                | 1   | 104–190     | 7.550 16 | 1 723.365 | 179.98 |
| 4-Chloroacetophenone             | 1   | 122–212     | 7.084 57 | 1 693.63  | 190.95 |
| Chloroacetyl chloride            | 1   | 28–107      | 7.149 77 | 1 340.79  | 208.70 |
| <i>N</i> -Chloroaniline          | 1   | 61–125      | 3.037 67 | 171.35    | –14.99 |
| 2-Chloroaniline                  | 1   | 20–108      | 7.562 65 | 1 998.6   | 220.0  |
|                                  | 1   | 108–300     | 7.192 40 | 1 762.74  | 200.0  |
| 3-Chloroaniline                  | 1   | 15–125      | 7.559 39 | 2 073.75  | 215    |
|                                  | 1   | 125–310     | 7.236 03 | 1 857.75  | 196.64 |
| <i>o</i> -Chloroanisole          | 1   | 115–186     | 7.121 36 | 1 655.80  | 188.77 |
| Chlorobenzene                    | 1   | 62–131.7    | 6.978 08 | 1 431.05  | 217.55 |
| <i>o</i> -Chlorobenzotrichloride | 1   | 30–150      | 7.504 30 | 2 228.07  | 220.0  |
|                                  | 1   | 150–350     | 7.117 94 | 1 951.37  | 196.27 |
| 1-Chloro-4-bromobenzene          | 2   | 23–63       | 11.629   | 3 643.30  |        |
| 1-Chlorobutane                   | 1   | –17 to 78.6 | 6.836 94 | 1 173.79  | 218.13 |
| 2-Chlorobutane                   | 1   | 0–40        | 6.799 23 | 1 149.12  | 224.68 |
| 1-Chlorodecane                   | 1   | 86–225.9    | 6.939 86 | 1 639.06  | 177.94 |
| 1-Chlorododecane                 | 1   | 116–246     | 6.834 08 | 1 654.82  | 155.09 |
| Chloroethane                     | 1   | –56 to 12.2 | 6.986 47 | 1 030.01  | 238.61 |
| 2-Chloroethylbenzene             | 1   |             | 6.981 69 | 1 556.0   | 201.0  |
| 3-Chloroethylbenzene             | 1   |             | 6.990 82 | 1 577.3   | 200    |
| 4-Chloroethylbenzene             | 1   |             | 6.983 09 | 1 577.0   | 200    |
| Chloroethylene                   | 1   | –65 to –13  | 6.891 17 | 905.01    | 239.48 |
| Chloroform                       | 1   | –35 to 61   | 6.493 4  | 929.44    | 196.03 |
| 1-Chloroheptane                  | 1   | 34–160      | 6.916 70 | 1 453.96  | 199.83 |
| 1-Chlorohexadecane               | 1   | 166–327     | 7.282 03 | 2 152.61  | 162.73 |
| 1-Chlorohexane                   | 1   | 15–136      | 7.051 36 | 1 461.72  | 215.57 |
| Chlorohexylisocyanate            | 1   | 90–180      | 7.740 95 | 2 340.50  | 241.90 |

TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                                     | Eq.            | Range, °C | A        | B         | C       |
|-----------------------------------------------|----------------|-----------|----------|-----------|---------|
| Chloromethane                                 | 1              | −75 to −5 | 7.093 49 | 948.58    | 249.34  |
| Chloromethoxytrichlorosilane                  | 1              | 0–50      | 7.312 92 | 1 545.71  | 226.10  |
| 2-Chloro-2-methylpropane                      | 1              | 22–47     | 4.896    | 334.99    | 114.0   |
| 1-Chlorononane                                | 1              | 69–205    | 7.046 54 | 1 655.57  | 192.26  |
| 1-Chlorooctane                                | 1              | 54–184    | 7.051 52 | 1 600.24  | 200.28  |
| Chloropentafluorobenzene                      | 1              | 36–140    | 7.068 83 | 1 389.19  | 213.75  |
| <i>p</i> -Chlorophenetole                     | 1              | 122–212   | 7.084 57 | 1 693.63  | 190.95  |
| 2-Chlorophenol                                | 1              | 80–200    | 6.877 31 | 1 471.61  | 193.17  |
| $\beta$ -Chloro- $\beta$ -phenylethyl alcohol | 1              | 166–259   | 6.917 33 | 1 635.63  | 145.87  |
| 1-Chlorophenylisocyanate                      | 1              | 50–160    | 12.265 9 | 6 532.55  | 499.59  |
| <i>m</i> -Chlorophenylisocyanate              | 1              | 71–158    | 6.797 29 | 1 512.43  | 180.90  |
| Chloroprene                                   | 1              | 20–60     | 6.161 50 | 783.45    | 179.7   |
| 1-Chloropropane                               | 1              | −25 to 47 | 6.926 48 | 1 110.19  | 227.94  |
| 2-Chloropropane                               | 1              | 0–30      | 7.771    | 1 582     | 288     |
| 3-Chloro-1-propene                            | 1              | 13–44     | 5.297 16 | 418.375   | 128.168 |
| 2-Chloropropionitrile                         | 1              | 0–84      | 7.329 73 | 1 732.55  | 211.79  |
|                                               | 1              | 84–240    | 7.200 85 | 1 657.25  | 205.3   |
| $\gamma$ -Chloropropyltrichlorosilane         | 1              | 87–179    | 7.156 4  | 1 679.07  | 210.38  |
| 1-Chlorotetradecane                           | 1              | 142–296.8 | 7.200 7  | 2 018.9   | 170.6   |
| <i>o</i> -Chlorotoluene                       | 1              | 0–65      | 7.367 97 | 1 735.8   | 230.0   |
|                                               | 1              | 65–220    | 6.947 63 | 1 497.2   | 209.0   |
| 1-Chloro-2,4,6-trinitrobenzene                | 1              | 200–270   | 3.080 9  | 184.93    | −117.9  |
| 1-Chloroundecane                              | 1              | 101–245   | 6.967 6  | 1 709.4   | 172.9   |
| <i>o</i> -Chlorovinylbenzene                  | 1              | 98–155    | 6.956 6  | 1 602.2   | 204.5   |
| <i>p</i> -Chlorovinylbenzene                  | 1              | 100–127   | 9.969 1  | 4 093.5   | 392.4   |
| 2-Chlorovinylchloroarsine                     | <i>cis</i> 1   | 68–109    | 5.487 9  | 785.09    | 115.61  |
|                                               | <i>trans</i> 1 | 50–150    | 6.814 0  | 1 465.07  | 178.53  |
| 3-Chlorovinylchloroarsine                     | 1              | 66–110    | 2.810 5  | 97.17     | −27.51  |
| <i>o</i> -Cresol                              | 1              | 120–191   | 6.911 7  | 1 435.50  | 165.16  |
| <i>m</i> -Cresol                              | 1              | 150–201   | 7.508 0  | 1 856.36  | 199.07  |
| <i>p</i> -Cresol                              | 1              | 128–202   | 7.035 08 | 1 511.08  | 161.85  |
| Cyanic acid                                   | 1              | −76 to −6 | 7.568 59 | 1 251.86  | 243.79  |
| Cyclobutane                                   | 1              | −60 to 12 | 6.916 31 | 1 054.54  | 241.37  |
| Cyclobutanone                                 | 1              | −24 to 25 | 6.116 68 | 933.95    | 183.19  |
| Cyclobutene                                   | 1              | −77 to 2  | 7.305 7  | 1 166.0   | 261.06  |
| Cycloheptane                                  | 1              | 68–159    | 6.853 95 | 1 331.57  | 216.35  |
| 1,3,5-Cycloheptatriene                        | 1              | 0–65      | 6.974 33 | 1 376.84  | 220.75  |
| Cyclohexane                                   | 1              | 20–81     | 6.841 30 | 1 201.53  | 222.65  |
| Cyclohexanethiol                              | 1              | 84–203    | 6.886 73 | 1 476.70  | 209.83  |
| Cyclohexanol                                  | 1              | 94–161    | 6.255 3  | 912.87    | 109.13  |
| Cyclohexene                                   | 1              |           | 6.886 17 | 1 229.973 | 224.10  |
| Cyclohexyl acetate                            | 1              | 95–172    | 7.975 86 | 2 167.99  | 252.30  |
| Cyclohexylamine                               | 1              | 61–128    | 6.689 54 | 1 229.42  | 188.80  |
| 1-Cyclohexylamino-2-propanol                  | 1              | 150–238   | 7.011 56 | 1 655.02  | 162.59  |
| Cyclohexylpentafluoropropionate               | 1              | 82–155    | 7.725 5  | 1 844.73  | 224.89  |
| Cyclohexyltrifluoroacetate                    | 1              | 72–147    | 7.802 35 | 1 954.66  | 249.33  |
| Cyclohexyltrimethylsilyl ether                | 1              | 91–168    | 8.090 52 | 2 276.62  | 267.94  |
| Cyclooctane                                   | 1              | 97–194    | 6.861 87 | 1 437.79  | 210.02  |
| 1,3,5,7-Cyclooctatetraene                     | 1              | 0–75      | 7.006 69 | 1 472.11  | 215.84  |
| Cyclopentane                                  | 1              | −40 to 72 | 6.886 76 | 1 124.162 | 231.36  |
| Cyclopentanethiol                             | 1              | 81–173    | 6.914 97 | 1 388.63  | 212.05  |
| Cyclopentanone                                | 1              | 0–26      | 2.902 47 | 162.90    | 63.22   |
| Cyclopentene                                  | 1              |           | 6.920 66 | 1 121.818 | 223.45  |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                     | Eq.          | Range, °C   | A        | B         | C       |
|-------------------------------|--------------|-------------|----------|-----------|---------|
| Cyclopentyl-1-thiaethane      | 1            | 83–199      | 6.940 83 | 1 480.70  | 208.47  |
| Cyclopropane                  | 1            | –90 to –32  | 6.887 88 | 856.01    | 246.50  |
| <i>o</i> -Cymene              | 1            | 81–180      | 7.266 10 | 1 768.45  | 224.95  |
| <i>m</i> -Cymene              | 1            | 79–176      | 7.123 74 | 1 644.95  | 212.76  |
| <i>p</i> -Cymene              | 1            | 107–178     | 7.050 74 | 1 608.91  | 208.72  |
| Decahydronaphthalene          | <i>cis</i>   | 68–228      | 6.875 29 | 1 594.460 | 203.39  |
|                               | <i>trans</i> | 61–219      | 6.856 81 | 1 564.683 | 206.26  |
| Decane                        | 1            | 58–203      | 6.943 65 | 1 495.17  | 193.86  |
| 1-Decanethiol                 | 1            | 109–271     | 6.998 1  | 1 713.6   | 177.0   |
| 1-Decanol                     | 1            | 25–52       | 11.560   | 4 055     | 273.2   |
|                               | 1            | 103–230     | 6.922 44 | 1 472.01  | 133.98  |
| 1-Decene                      | 1            | 54–199      | 6.934 77 | 1 484.98  | 195.707 |
| Decylbenzene                  | 1            | 203–298     | 7.035 96 | 1 903.98  | 160.33  |
| Decylcyclohexane              | 1            | 197–298     | 7.019 37 | 1 899.33  | 161.35  |
| Decylcyclopentane             | 1            | 182–279     | 6.999 12 | 1 822.05  | 163.05  |
| Deuterodiborane               | 1            | –155 to –94 | 6.480 83 | 545.20    | 244.73  |
| Diacetone alcohol             | 1            | 28–115      | 8.502 42 | 2 400.56  | 263.79  |
| 1,3-Diacetylbenzene           | 1            | 50–145      | 0.056 24 | 64.188    | –196.97 |
| 1,4-Diacetylbenzene           | 1            | 116–157     | 2.803 71 | 177.25    | –46.43  |
| Diacetylene                   | 1            | –78 to 0    | 4.990 79 | 356.36    | 143.22  |
| Diallyl sulfide               | 1            | 10–40       | 4.829 30 | 643.18    | 142.34  |
| 4,4'-Diaminodiphenylmethane   | 1            | 198–272     | 3.172 31 | 210.49    | –137.41 |
| Diamyl ether                  | 1            | 105–187     | 7.067 10 | 1 604.77  | 196.58  |
| Dibenzyl ketone               | 2            | 285–325     | 8.257    | 3 244.42  |         |
| 1,2-Dibromobenzene            | 1            | 20–117      | 7.501 28 | 2 093.7   | 230     |
|                               | 1            | 117–300     | 7.102 65 | 1 825.77  | 207.0   |
| Dibromodichloroethane         | 1            | 25–130      | 5.197 53 | 763.44    | 110.81  |
| Dibromodifluoromethane        | 1            | –26 to 23   | 7.152 22 | 1 181.612 | 253.85  |
| 1,2-Dibromoethane             | 1            | 52–131      | 6.721 48 | 1 280.82  | 201.75  |
| 1,2-Dibromoethylene           | <i>cis</i>   | 26–78       | 7.038 74 | 1 349.84  | 209.26  |
|                               | <i>trans</i> | 4–71        | 4.581 11 | 393.641   | 103.56  |
| 1,2-Dibromopropane            | 1            | 0–50        | 7.303 98 | 1 644.4   | 232.0   |
|                               | 1            | 50–250      | 6.891 05 | 1 419.60  | 212.0   |
| 1,3-Dibromopropane            | 1            | 0–71        | 7.549 84 | 1 890.56  | 240.0   |
|                               | 1            | 71–275      | 7.198 74 | 1 678.26  | 222.0   |
| Di- <i>n</i> -butyl ether     | 1            | 89–140      | 6.796 3  | 1 297.29  | 191.03  |
| Di- <i>t</i> -butyl ether     | 1            | 4–109       | 6.932 9  | 1 348.53  | 233.79  |
| Di- <i>n</i> -butyl phthalate | 1            | 126–202     | 6.639 80 | 1 744.20  | 113.69  |
| Di- <i>n</i> -butyl sebacate  | 1            | 128–208     | 7.587 66 | 2 364.89  | 147.54  |
| Di- <i>n</i> -butyl sulfide   | 1            | 10–40       | 6.769 3  | 1 208.80  | 217.51  |
| 1,2-Dichlorobenzene           | 1            | 131–181     | 7.143 78 | 1 704.49  | 219.42  |
| 1,3-Dichlorobenzene           | 1            | 91–173      | 7.040 1  | 1 607.05  | 213.38  |
| 1,4-Dichlorobenzene           | 1            | 95–174      | 7.020 8  | 1 590.9   | 210.2   |
| Dichlorobenzotrichloride      | 1            | 20–167      | 7.439 54 | 2 190.0   | 200     |
|                               | 1            | 167–340     | 6.985 24 | 1 868.91  | 172.00  |
| Dichlorobenzyl chloride       | 1            | 20–138      | 7.504 57 | 2 125.9   | 213.8   |
|                               | 1            | 138–350     | 7.147 35 | 1 881.38  | 192.93  |
| 1,1-Dichloroethane            | 1            | –39 to 18   | 6.977 0  | 1 174.02  | 229.06  |
| 1,2-Dichloroethane            | 1            | –31 to 99   | 7.025 3  | 1 271.3   | 222.9   |
| 1,1-Dichloroethylene          | 1            | –28 to 32   | 6.972 2  | 1 099.4   | 237.2   |
| 1,2-Dichloroethylene          | <i>cis</i>   | 0–84        | 7.022 3  | 1 205.4   | 230.6   |
|                               | <i>trans</i> | –38 to 85   | 6.965 1  | 1 141.9   | 231.9   |
| 2,2'-Dichloroethyl sulfide    | 1            | 15–76       | 8.587 41 | 2 588.23  | 246.06  |



TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                                        | Eq. | Range, °C   | A        | B         | C       |
|--------------------------------------------------|-----|-------------|----------|-----------|---------|
| 1,2-Dichloroethyltrichlorosilane                 | 1   | 102–181     | 7.826    | 2 144.9   | 253.1   |
| Dichloromethane                                  | 1   | –40 to 40   | 7.409 2  | 1 325.9   | 252.6   |
| 2-(2,4-Dichlorophenoxy)-ethanol                  | 1   | 212–286     | 7.240 09 | 2 004.31  | 157.25  |
| 3,4-Dichlorophenylisocyanate                     | 1   | 60–190      | 8.679 3  | 3 312.3   | 333.9   |
| 1,2-Dichloropropane                              | 1   | 45–96       | 6.980 7  | 1 308.1   | 222.8   |
| 3,4-Dichlorotoluene                              | 1   | 0–105       | 7.343 94 | 1 882.5   | 215.0   |
|                                                  | 1   | 105–330     | 6.979 25 | 1 655.44  | 195.0   |
| Diethanolamine                                   | 1   | 194–241     | 8.138 8  | 2 327.9   | 174.4   |
| 1,1-Diethoxyethane                               | 1   | 0–70        | 6.757 63 | 1 191.60  | 203.12  |
| Diethoxymethane                                  | 1   | 0–75        | 6.908 41 | 1 229.52  | 217.01  |
| Diethylaluminum chloride                         | 1   | 44–125      | 8.229 70 | 2 484.53  | 255.45  |
| Diethylamine                                     | 1   | 31–61       | 5.801 6  | 583.30    | 144.1   |
| N,N-Diethylaniline                               | 1   | 50–218      | 7.466 0  | 1 993.57  | 218.5   |
| 1,2-Diethylbenzene                               | 1   | liq         | 6.987 80 | 1 576.940 | 200.51  |
| 1,3-Diethylbenzene                               | 1   | liq         | 7.003 60 | 1 575.310 | 200.96  |
| 1,4-Diethylbenzene                               | 1   | liq         | 6.998 20 | 1 588.310 | 201.97  |
| Diethyldichlorosilane                            | 1   | 48–128      | 6.862 9  | 1 346.3   | 207.7   |
| Diethyl disulfide                                | 1   | 15–61       | 7.349 89 | 1 695.00  | 227.29  |
|                                                  | 1   | 61–230      | 6.975 07 | 1 485.970 | 208.96  |
| Diethylene glycol                                | 1   | 130–243     | 7.636 7  | 1 939.4   | 162.7   |
| Diethyl ether                                    | 1   | –61 to 20   | 6.920 32 | 1 064.07  | 228.80  |
| Diethyl ethylphosphate                           | 1   | 76–134      | 4.101 6  | 315.17    | 15.50   |
| N,N-Diethylformamide                             | 1   | 30–90       | 6.395 4  | 1 203.8   | 165.6   |
| Diethyl ketone                                   | 1   |             | 6.857 91 | 1 216.3   | 204     |
| 3,3-Diethylpentane                               | 1   | 63–147      | 6.896 03 | 1 453.48  | 215.83  |
| 3,5-Diethylphenol                                | 1   | 114–248     | 7.651 3  | 2 228     | 218.5   |
| Diethylpropylphosphonate                         | 1   | 87–134      | 4.558 1  | 446.50    | 26.17   |
| Diethyl sulfide                                  | 1   | 0–150       | 6.928 36 | 1 257.83  | 218.66  |
| 1,2-bis-Difluoroamino-4-methyl-pentane           | 1   | –20 to 20   | 8.009 11 | 1 944.92  | 245.44  |
| Difluoromethane                                  | 1   | –82 to –32  | 7.138 9  | 821.7     | 244.7   |
| 1,2-Dihydroxybenzene                             | 1   | 118–246     | 7.577    | 2 054     | 187     |
| 1,3-Dihydroxybenzene                             | 1   | 151–276     | 7.889    | 2 231     | 169     |
| 1,2-Diiodoethylene <i>cis</i>                    | 1   | 29–152      | 5.522    | 797.8     | 106.4   |
| <i>trans</i>                                     | 1   | 77–130      | 6.093 1  | 1 197.0   | 172.3   |
| Diisoamyl sulfide                                | 1   | 10–80       | –1.959 8 | 390.61    | –219.33 |
| p-Diisopropylbenzene                             | 1   | 120–211     | 6.993 3  | 1 663.88  | 194.41  |
| Diisopropyl ether                                | 1   | 23–67       | 6.849 5  | 1 139.34  | 218.7   |
| 2,4-Diisopropylphenol                            | 1   | 122–255     | 6.714    | 1 506     | 138     |
| 1,2-Dimethoxyethane                              | 1   | 0–60        | 6.718 9  | 1 050.5   | 209.2   |
| N,N-Dimethylacetamide                            | 1   | 30–90       | 9.720 9  | 3 273.8   | 334.5   |
| Dimethylamine                                    | 1   | –72 to 6.9  | 7.082 12 | 960.242   | 221.67  |
| bis-Dimethylaminoborane                          | 1   | –25 to 62.5 | 5.584 52 | 774.371   | 170.64  |
| N-Dimethylaminodiborane                          | 1   | –38 to 14   | 8.340 1  | 1 917.35  | 302.73  |
| bis-Dimethylaminodifluorosilane                  | 1   | 24–88       | 5.952    | 748.7     | 146.9   |
| N,N-Dimethylaniline                              | 1   | 71–197      | 7.367 7  | 1 857.08  | 220.36  |
| Dimethyl beryllium                               | 1   | 100–180     | 19.089 9 | 11 535.45 | 496.64  |
| 1,4-Dimethyl-bicyclo(2,2,1)-heptane              | 1   | 56–119      | 6.761 96 | 1 342.66  | 213.53  |
| 2,3-Dimethyl-bicyclo(2,2,1)-heptane <i>trans</i> | 1   | 72–138      | 6.868 15 | 1 420.32  | 212.94  |
| 2,3-Dimethyl-1,3-butadiene                       | 1   | 0–68.5      | 7.119 7  | 1 299.69  | 238.09  |
| 2,2-Dimethylbutane                               | 1   | –42 to 73   | 6.754 83 | 1 081.176 | 229.34  |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                         | Eq.          | Range, °C   | A        | B         | C      |
|-----------------------------------|--------------|-------------|----------|-----------|--------|
| 2,3-Dimethylbutane                | 1            | −35 to 81   | 6.809 83 | 1 127.187 | 228.90 |
| 2,3-Dimethyl-2-butanethiol        | 1            | 56–167      | 6.839 56 | 1 354.24  | 215.96 |
| 2,3-Dimethyl-1-butene             | 1            | −36 to 78   | 6.862 36 | 1 134.675 | 229.37 |
| 2,3-Dimethyl-2-butene             | 1            | −21 to 97   | 6.950 58 | 1 215.428 | 225.44 |
| 3,3-Dimethyl-1-butene             | 1            | −47 to 64   | 6.677 51 | 1 010.516 | 224.91 |
| Dimethyl cadmium                  | 1            | −2 to 23    | 6.490 55 | 1 126.36  | 201.07 |
| 1,1-Dimethylcyclohexane           | 1            | 10–147      | 6.798 21 | 1 321.705 | 217.85 |
| 1,2-Dimethylcyclohexane           | <i>cis</i>   | 18–158      | 6.837 46 | 1 367.311 | 215.84 |
|                                   | <i>trans</i> | 13–151      | 6.833 08 | 1 353.881 | 219.13 |
| 1,3-Dimethylcyclohexane           | <i>cis</i>   | 11–147      | 6.838 83 | 1 338.473 | 218.07 |
|                                   | <i>trans</i> | 15–152      | 6.834 55 | 1 343.687 | 215.39 |
| 1,4-Dimethylcyclohexane           | <i>cis</i>   | 15–152      | 6.832 87 | 1 345.613 | 216.15 |
|                                   | <i>trans</i> | 10–147      | 6.817 73 | 1 330.437 | 218.58 |
| 1,1-Dimethylcyclopentane          | 1            | −12 to 113  | 6.817 24 | 1 219.474 | 221.95 |
| 1,2-Dimethylcyclopentane          | <i>cis</i>   | −3 to 125   | 6.850 08 | 1 269.140 | 220.21 |
|                                   | <i>trans</i> | −9 to 117   | 6.844 22 | 1 242.748 | 221.69 |
| 1,3-Dimethylcyclopentane          | <i>cis</i>   | −10–116     | 6.837 15 | 1 237.456 | 222.01 |
|                                   | <i>trans</i> | −9 to 117   | 6.838 17 | 1 240.023 | 221.62 |
| Dimethyldichlorosilane            | 1            | 28–72       | 7.062 1  | 1 280.29  | 235.65 |
| 1,2-Dimethyldisilane              | 1            | −46 to 0    | 4.024 3  | 255.4     | 129.2  |
| Dimethyl ether                    | 1            | −71 to −25  | 6.976 03 | 889.264   | 241.96 |
| <i>N,N</i> -Dimethylformamide     | 1            | 30–90       | 6.928 0  | 1 400.87  | 196.43 |
| 2,2-Dimethylhexane                | 1            |             | 6.837 15 | 1 273.59  | 215.07 |
| 2,3-Dimethylhexane                | 1            |             | 6.870 04 | 1 315.50  | 214.16 |
| 2,4-Dimethylhexane                | 1            |             | 6.853 05 | 1 287.88  | 214.79 |
| 2,5-Dimethylhexane                | 1            |             | 6.859 84 | 1 287.27  | 214.41 |
| 3,3-Dimethylhexane                | 1            |             | 6.851 21 | 1 307.88  | 217.44 |
| 3,4-Dimethylhexane                | 1            |             | 6.879 86 | 1 330.04  | 214.86 |
| 1,1-Dimethylhydrazine             | 1            | −35 to 20   | 7.408 13 | 1 305.91  | 225.53 |
| 1,2-Dimethylhydrazine             | 1            | 1–25        | 5.611 9  | 633.59    | 143.17 |
| <i>N,N</i> -Dimethylhydroxylamine | 1            | 17–90       | 7.565 8  | 1 415.96  | 201.93 |
| <i>O,N</i> -Dimethylhydroxylamine | 1            | −45 to 42.2 | 7.405 4  | 1 245.58  | 233.06 |
| Dimethylmalononitrile             | 1            | 49–140      | 7.035 5  | 1 546.99  | 202.00 |
| 1,3-Dimethylnaphthalene           | 1            | 20–148      | 7.634 7  | 2 295.4   | 232.4  |
|                                   | 1            | 148–310     | 7.269 8  | 2 076.0   | 210    |
| 1,4-Dimethylnaphthalene           | 1            | 20–148      | 7.634 7  | 2 345.8   | 232.6  |
| (same for 1,6- and 1,7-)          | 1            | 148–310     | 7.269 8  | 2 076.0   | 210    |
| 1,8-Dimethylnaphthalene           | 1            | 25–150      | 7.407 89 | 2 123.2   | 201.2  |
|                                   | 1            | 150–320     | 7.056 4  | 1 879     | 180    |
| 2,3-Dimethylnaphthalene           | 1            | 20–155      | 7.403 96 | 2 111.9   | 201.1  |
|                                   | 1            | 155–315     | 7.052 7  | 1 869     | 180    |
| 2,6-Dimethylnaphthalene           | 1            | 20–150      | 7.396 8  | 2 080.3   | 200.8  |
|                                   | 1            | 150–310     | 7.046 0  | 1 841     | 180    |
| 2,7-Dimethylnaphthalene           | 1            | 25–150      | 7.398 75 | 2 085.9   | 200.9  |
|                                   | 1            | 150–310     | 7.047 8  | 1 846     | 180    |
| 2,2-Dimethylpentane               | 1            | −19 to 103  | 6.814 80 | 1 190.033 | 223.30 |
| 2,3-Dimethylpentane               | 1            | −10 to 115  | 6.853 82 | 1 238.017 | 221.82 |
| 2,4-Dimethylpentane               | 1            | −17 to 105  | 6.826 21 | 1 192.04  | 225.32 |
| 3,3-Dimethylpentane               | 1            | −14 to 112  | 6.826 67 | 1 228.663 | 225.32 |
| 2,4-Dimethyl-3-pentanone          | 1            | 48–125      | 6.968 53 | 1 382.84  | 213.06 |
| Dimethyl- <i>o</i> -phthalate     | 1            | 82–151      | 4.522 32 | 700.31    | 51.42  |
| 2,2-Dimethylpropane               | 1            | −14 to 29   | 6.604 27 | 883.42    | 227.78 |
| 2,2-Dimethyl-1-propanol           | 1            | 55–115      | 7.875 3  | 1 604.7   | 208.2  |

TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                    | Eq. | Range, °C   | A        | B         | C      |
|------------------------------|-----|-------------|----------|-----------|--------|
| 2,5-Dimethylpyrrole          | 1   | 100–199     | 7.203 06 | 1 509.60  | 181.76 |
| 2,4-Dimethylquinoline        | 1   | 185–269     | 7.025 4  | 1 830.29  | 174.44 |
| 2,6-Dimethylquinoline        | 1   | 188–267     | 6.931 12 | 1 748.73  | 166.37 |
| Dimethyl sulfide             | 1   | –22 to 20   | 7.150 9  | 1 195.58  | 242.68 |
| 3,3-Dimethyl-2-thiabutane    | 1   | liq         | 6.847 09 | 1 259.648 | 218.69 |
| 2,2-Dimethyl-3-thiapentane   | 1   | liq         | 6.850 86 | 1 323.24  | 212.89 |
| 2,4-Dimethyl-3-thiapentane   | 1   | liq         | 6.871 18 | 1 327.12  | 212.55 |
| 2,3-Dimethylthiophene        | 1   | 50–205      | 6.924 9  | 1 430.0   | 212    |
| 2,4-Dimethylthiophene        | 1   | 50–205      | 6.993 9  | 1 450.7   | 212.0  |
| 2,5-Dimethylthiophene        | 1   | 47–200      | 6.961 1  | 1 427.7   | 213.2  |
| 3,4-Dimethylthiophene        | 1   | 54–205      | 6.996 1  | 1 467.1   | 211.5  |
| 1,3-Dinitrobenzene           | 1   | 252–292     | 4.337    | 229.2     | –137   |
| 2,4-Dinitrotoluene           | 1   | 200–299     | 5.798    | 1 118     | 61.8   |
| 2,6-Dinitrotoluene           | 1   | 150–260     | 4.372    | 380       | –43.6  |
| 3,5-Dinitrotoluene           | 1   | 220–270     | 1.556    | 30.59     | –302   |
| 1,4-Dioxane                  | 1   | 20–105      | 7.431 55 | 1 554.68  | 240.34 |
| Dipentene                    | 1   | 21–170      | 7.111 6  | 1 613.42  | 207.8  |
| 2,2'-Diphenol                | 1   | 171–325     | 8.193 5  | 3 067.6   | 253.1  |
| Diphenyldichlorosilane       | 1   | 192–281     | 6.999 03 | 1 918.20  | 161.41 |
| Diphenyl ether               | 1   | 204–271     | 7.011 04 | 1 799.71  | 177.74 |
| Diphenylmethane              | 1   | 217–282     | 6.291    | 1 261     | 105    |
| Di- <i>n</i> -propyl ether   | 1   | 26–89       | 6.947 6  | 1 256.5   | 219.0  |
| Disilanyl chloride           | 1   | –46 to 18   | 7.104 8  | 1 211.8   | 245.2  |
| 2,3-Dithiabutane             | 1   | 6–135       | 6.977 92 | 1 346.342 | 218.86 |
| 5,6-Dithiadecane             | 1   | 101–263     | 6.963 8  | 1 684.1   | 181.3  |
| 3,4-Dithiahexane             | 1   | 40–182      | 6.975 07 | 1 485.970 | 208.96 |
| 4,5-Dithiaoctane             | 1   | 72–226      | 6.975 29 | 1 603.793 | 195.85 |
| Dodecane                     | 1   | 91–247      | 6.997 95 | 1 639.27  | 181.84 |
| 1-Dodecanethiol              | 1   |             | 7.024 4  | 1 817.8   | 164.1  |
| Dodecanoic acid              | 1   | 106–176     | 7.860 8  | 2 159.1   | 143.2  |
| 1-Dodecanol                  | 1   | 138–214     | 7.539 86 | 2 003.29  | 168.13 |
| 1-Dodecene                   | 1   | 89–244      | 6.976 07 | 1 621.11  | 182.45 |
| Durenol                      | 1   | 108–249     | 7.758    | 2 432     | 250    |
| Eicosane                     | 1   | 198–379     | 7.152 2  | 2 032.7   | 132.1  |
| 1-Eicosanethiol              | 1   |             | 7.114    | 2 125     | 119    |
| 1-Eicosene                   | 1   | liq         | 7.135 1  | 2 043.0   | 137.9  |
| Ethane                       | 1   | –142 to –75 | 6.829 15 | 663.72    | 256.68 |
| Ethanethiol                  | 1   | –49 to 56   | 6.952 06 | 1 084.531 | 231.39 |
| Ethanol                      | 1   | –2 to 100   | 8.321 09 | 1 718.10  | 237.52 |
| Ethanolamine                 | 1   | 65–171      | 7.456 8  | 1 577.67  | 173.37 |
| Ethyl acetate                | 1   | 15–76       | 7.101 79 | 1 244.95  | 217.88 |
| <i>m</i> -Ethylacetophenone  | 1   | 19–143      | 3.767 2  | 708.05    | 182.6  |
| <i>p</i> -Ethylacetophenone  | 1   | 21–94       | 4.274 6  | 629.34    | 120.9  |
| Ethylamine                   | 1   | –20 to 90   | 7.054 13 | 987.31    | 220.0  |
| <i>N</i> -Ethylaniline       | 1   | 50–207      | 7.422 8  | 1 903.4   | 214.3  |
| Ethylbenzene                 | 1   | 26–164      | 6.957 19 | 1 424.255 | 213.21 |
| 2-Ethyl-1-butene             | 1   | –28 to 88   | 6.997 12 | 1 218.352 | 231.30 |
| Ethyl butyl ether            | 1   | 38–92       | 6.944 4  | 1 256.4   | 216.9  |
| Ethyl chloroacetate          | 1   | 25–146      | 6.967    | 1 355.9   | 188.2  |
| <i>p</i> -Ethylchlorobenzene | 1   | 109–184     | 6.951 1  | 1 557.1   | 198.1  |
| Ethylcyclohexane             | 1   | 20–160      | 6.867 28 | 1 382.466 | 214.99 |
| Ethylcyclopentane            | 1   | –0.1 to 129 | 6.887 09 | 1 298.599 | 220.68 |
| Ethylene                     | 1   | –153 to –91 | 6.744 19 | 594.99    | 256.16 |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                             | Eq. | Range, °C   | A        | B         | C      |
|---------------------------------------|-----|-------------|----------|-----------|--------|
| Ethylene glycol                       | 1   | 50–200      | 8.090 8  | 2 088.9   | 203.5  |
| Ethylene glycol monoethyl ether       | 1   | 63–134      | 7.874 6  | 1 843.5   | 234.2  |
| Ethylene glycol monomethyl ether      | 1   | 56–124      | 7.849 8  | 1 793.9   | 236.9  |
| Ethylene oxide                        | 1   | –49 to 12   | 7.128 43 | 1 054.54  | 237.76 |
| Ethyl formate                         | 1   | 4–54        | 7.009 0  | 1 123.94  | 218.2  |
| 3-Ethylhexane                         | 1   |             | 6.890 98 | 1 327.88  | 212.60 |
| 2-Ethyl-1-hexanol                     | 1   | 74–184      | 6.914 7  | 1 339.7   | 147.8  |
| 2-Ethyl-2-hexenal                     | 1   | 54–175      | 6.861 3  | 1 457.4   | 190.6  |
| Ethyl iodoacetate                     | 1   | 29–89       | 4.073 7  | 374.64    | 54.8   |
| Ethyl isothiocyanate                  | 1   | 10–50       | 7.106 0  | 1 567.5   | 234.2  |
| Ethyl methyl ether                    | 1   | 5–7.7       | 5.518    | 434.5     | 158    |
| Ethyl methyl ketone                   | 1   |             | 6.974 21 | 1 209.6   | 216    |
| 3-Ethyl-5-methylphenol                | 1   | 195–247     | 7.040 83 | 1 615.44  | 152.6  |
| 2-Ethyl-4-methyl-1-pentanol           | 1   | 70–176      | 6.582 6  | 1 134.6   | 129.2  |
| Ethyl nitrate                         | 1   | 0–60        | 7.163 7  | 1 338.8   | 224.9  |
| 3-Ethylpentane                        | 1   | –7 to 119   | 6.875 64 | 1 251.827 | 219.89 |
| 2-Ethylphenol                         | 1   | 86–208      | 7.800 3  | 2 140.4   | 227    |
| 3-Ethylphenol                         | 1   | 97–218      | 7.468    | 1 856     | 187    |
| 4-Ethylphenol                         | 1   | 101–218     | 8.291    | 2 423     | 229    |
| Ethyl phenyl ether                    | 1   | 117–181     | 7.021 38 | 1 508.39  | 194.49 |
| Ethyl <i>n</i> -propanoate            | 1   | 34–98       | 6.994 9  | 1 260.6   | 207.4  |
| Ethyl <i>n</i> -propyl ether          | 1   | 20–63       | 6.985 1  | 1 188.5   | 226.4  |
| Ethyl <i>n</i> -propyl ketone         | 1   | 75–133      | 7.000 82 | 1 365.79  | 208.01 |
| <i>m</i> -Ethylstyrene                | 1   |             | 7.039 28 | 1 614.0   | 198    |
| <i>p</i> -Ethylstyrene                | 1   |             | 6.900 71 | 1 570.9   | 198    |
| Ethyl trichloroacetate                | 1   | 44–95       | 7.725 4  | 1 927.0   | 233.7  |
| Ethyl trichlorosilane                 | 1   | 28–96       | 6.606    | 1 118     | 201    |
| Ethyl triethoxysilane                 | 1   | 64–153      | 6.886 8  | 1 377.9   | 183.0  |
| Ethyl vinylchlorosilane               | 1   | 45–122      | 6.859    | 1 331     | 210.8  |
| Fenchyl alcohol                       | 1   | 59–200      | 5.693    | 797.6     | 84.6   |
| Fluoranthene                          | 1   | 197–384     | 6.373    | 1 756     | 118    |
| Fluorene                              | 1   | 161–300     | 7.761 8  | 2 637.1   | 243.2  |
| Fluorobenzene                         | 1   | –18 to 84   | 7.187 0  | 1 381.8   | 235.6  |
| <i>m</i> -Fluorobenzotrifluoride      | 1   | 40–137      | 7.006 59 | 1 304.35  | 215.67 |
| <i>bis</i> -(Fluorocarbonyl)-peroxide | 1   | –47 to –7   | 9.608 4  | 2 247.64  | 319.83 |
| <i>p</i> -Fluorotoluene               | 1   | 68–155      | 6.994 26 | 1 374.055 | 217.40 |
| Formaldehyde                          | 1   | –109 to –22 | 7.195 8  | 970.6     | 244.1  |
| Formic acid                           | 1   | 37–101      | 7.581 8  | 1 699.2   | 260.7  |
| Formyl fluoride                       | 1   | –95 to –61  | 5.270    | 362       | 175    |
| Furan                                 | 1   | 2–61        | 6.975 27 | 1 060.87  | 227.74 |
| 2-Furfuraldehyde                      | 1   | 56–161      | 6.575 9  | 1 198.7   | 162.8  |
| Glycerol                              | 1   | 183–260     | 6.165    | 1 036     | 28     |
| Glyceryl-1,3-diacetate                | 1   | 100–190     | 6.407 3  | 1 092.0   | 119.3  |
| Guaiacol                              | 1   | 82–205      | 6.161    | 1 051     | 116    |
| Hemellitenol                          | 1   | 123–248     | 6.972    | 1 563     | 134    |
| Heptadecane                           | 1   | 161–337     | 7.014 3  | 1 865.1   | 149.20 |
| 1-Heptadecene                         | 1   |             | 7.008 67 | 1 868.9   | 152.50 |
| Heptane                               | 1   | –2 to 124   | 6.896 77 | 1 264.90  | 216.54 |
| 1-Heptanethiol                        | 1   | 58–206      | 6.952 49 | 1 525.311 | 197.70 |
| Heptanoic acid                        | 1   | 112–150     | 5.287 4  | 665.54    | 42.07  |
| 1-Heptanol                            | 1   | 60–176      | 6.647 67 | 1 140.64  | 126.56 |
| 1-Heptene                             | 1   | –6 to 118   | 6.901 87 | 1 258.345 | 219.30 |
| Hexadecane                            | 1   | 149–321     | 7.028 67 | 1 830.51  | 154.45 |

TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                       | Eq. | Range, °C  | A        | B         | C      |
|---------------------------------|-----|------------|----------|-----------|--------|
| 1-Hexadecanethiol               | 1   |            | 7.075    | 1 990     | 140    |
| 1-Hexadecanol                   | 1   | 50–103     | 7.281 7  | 1 909.7   | 128.1  |
|                                 | 1   | 145–190    | 6.158 6  | 1 380.0   | 91     |
| 1-Hexadecene                    | 1   |            | 7.040 11 | 1 840.52  | 157.57 |
| 1,5-Hexadiene                   | 1   | 0–59       | 6.574 1  | 1 013.5   | 214.8  |
| Hexafluoroacetone               | 1   | –79 to –27 | 6.650 2  | 725.90    | 219.9  |
| Hexafluorobenzene               | 1   | 5–114      | 7.032 95 | 1 227.98  | 215.49 |
| Hexafluorodisiloxane            | 1   | –39 to –23 | 7.471 2  | 1 169.3   | 278.1  |
| Hexafluoroethane                | 1   | –93 to –78 | 6.793 35 | 657.06    | 246.2  |
| Hexahydroindane <i>cis</i>      | 1   | 77–168     | 6.868 22 | 1 497.33  | 207.67 |
| <i>trans</i>                    | 1   | 71–161     | 6.861 19 | 1 475.70  | 209.66 |
| Hexamethyldisiloxane            | 1   | 36–138     | 6.773 79 | 1 202.03  | 208.25 |
| Hexane                          | 1   | –25 to 92  | 6.876 01 | 1 171.17  | 224.41 |
| 1-Hexanethiol                   | 1   | 40–181     | 6.946 64 | 1 454.004 | 204.95 |
| 1-Hexanol                       | 1   | 35–157     | 7.860 45 | 1 761.26  | 196.66 |
| 2-Hexanol                       | 1   | 25–142     | 7.261 0  | 1 371.7   | 173.2  |
| 3-Hexanol                       | 1   | 25–138     | 7.689    | 1 670.0   | 211.8  |
| 1-Hexene                        | 1   | 16–64      | 6.857 70 | 1 148.62  | 225.35 |
| 3-Hexyne                        | 1   | –20 to 24  | 5.895    | 863.3     | 194    |
| Hydroquinone                    | 1   | 159–286    | 8.137    | 2 461     | 183    |
| 3-Hydroxy-3-methyl-2-butanone   | 1   | 45–146     | 7.340 9  | 1 653.6   | 227.5  |
| Iodobenzene                     | 1   | 20–188     | 7.011 9  | 1 640.1   | 208.8  |
| Iodoethane                      | 1   | 30–60      | 6.959    | 1 232     | 229    |
| Isoamyl acetate                 | 1   | 41–95      | 7.436    | 1 606.6   | 216    |
| Isobutylbenzene                 | 1   | 86–174     | 6.935 56 | 1 530.05  | 204.59 |
| Isobutyl borate                 | 1   | 99–200     | 7.197    | 1 745.8   | 193    |
| Isobutyl cellosolve             | 1   | 71–159     | 7.694 8  | 1 825.9   | 219.6  |
| Isobutylcyclohexane             | 1   | 85–172     | 6.867 97 | 1 493.10  | 203.16 |
| Isobutyl nitrate                | 1   | 0–70       | 8.164 3  | 2 022.7   | 262.4  |
| Isobutyraldehyde                | 1   | 13–63      | 6.735 1  | 1 053.2   | 209.1  |
| Isobutyric acid                 | 1   | 58–152     | 4.894    | 382.6     | 38     |
| Isocaproic acid                 | 1   | 96–133     | 6.258    | 1 038.6   | 130    |
| Isopropylbenzene                | 1   | 39–181     | 6.936 66 | 1 460.793 | 207.78 |
| Isopropyl borate                | 1   | 65–139     | 8.070    | 2 120     | 269    |
| <i>o</i> -Isopropylbromobenzene | 1   | 132–210    | 6.717 8  | 1 462.7   | 170.9  |
| Isopropyl caprate               | 1   | 90–178     | 9.959    | 4 013.9   | 326.5  |
| Isopropyl caprylate             | 1   | 65–146     | 8.032 2  | 2 213.6   | 220.9  |
| Isopropyl cellosolve            | 1   | 67–140     | 7.500 0  | 1 639.2   | 213.3  |
| Isopropyl chloroacetate         | 1   | 35–153     | 8.382    | 2 328     | 275    |
| Isopropylcyclohexane            | 1   | 71–155     | 6.873 14 | 1 453.20  | 209.44 |
| Isopropylcyclopentane           | 1   | 47–127     | 6.887 36 | 1 380.12  | 218.05 |
| Isopropyl laurate               | 1   | 117–196    | 8.532 6  | 2 951.6   | 240.7  |
| Isopropyl myristate             | 1   | 140–193    | 10.418 0 | 4 866.48  | 314.17 |
| Isopropyl nitrate               | 1   | 0–70       | 7.266 6  | 1 434.4   | 255.2  |
| Isopropyl palmitate             | 1   | 160–197    | 10.916 4 | 5 572.0   | 364.8  |
| <i>o</i> -Isopropylphenol       | 1   | 97–215     | 8.167    | 2 343     | 229    |
| <i>p</i> -Isopropylphenol       | 1   | 108–228    | 8.666    | 2 810     | 258    |
| Isopropyl phenyl ether          | 1   | 72–175     | 6.517 6  | 1 238.0   | 163.0  |
| Isopropyl stearate              | 1   | 182–207    | 0.079 3  | 10.41     | –221   |
| Isopseudocumenol                | 1   | 106–233    | 5.602    | 768       | 49     |
| Isoquinoline                    | 1   | 167–244    | 6.912 2  | 1 723.4   | 184.3  |
| Isovaleric acid                 | 1   | 86–104     | 3.946 55 | 255.41    | 11.3   |
| Ketene                          | 1   | –88 to –49 | 7.615    | 1 036     | 269    |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                 | Eq. | Range, °C    | A        | B         | C      |
|---------------------------|-----|--------------|----------|-----------|--------|
| Lauric acid               | 1   | 106–176      | 7.860 8  | 2 159.1   | 143.2  |
| Lepidine                  | 1   | 199–266      | 7.271 2  | 1 946.14  | 177.64 |
| 2,3-Lutidine              | 1   | 155–162      | 7.447 8  | 1 832.6   | 240.1  |
| 2,4-Lutidine              | 1   | 150–160      | 7.339 0  | 1 733.4   | 230.4  |
| 2,5-Lutidine              | 1   | 85–157       | 7.081 0  | 1 539.6   | 209.6  |
| 2,6-Lutidine              | 1   | 79–144       | 7.056 7  | 1 470.2   | 208.0  |
| 3,4-Lutidine              | 1   | 172–180      | 7.362 0  | 1 840.1   | 231.5  |
| 3,5-Lutidine              | 1   | 163–173      | 7.333 1  | 1 783.6   | 228.7  |
| Mesitol                   | 1   | 94–221       | 6.659    | 1 392     | 148    |
| Mesityl oxide             | 1   | 14–130       | 6.635 8  | 1 186.1   | 186.0  |
| Methacrylonitrile         | 1   |              | 6.980 2  | 1 274.96  | 220.7  |
| Methane c                 | 1   | –195 to –183 | 7.193 09 | 451.64    | 268.49 |
| liq                       | 1   | –181 to –152 | 6.695 61 | 405.42    | 267.78 |
| Methanol                  | 1   | –14 to 65    | 7.897 50 | 1 474.08  | 229.13 |
|                           | 1   | 64–110       | 7.973 28 | 1 515.14  | 232.85 |
| Methoxybenzene            | 1   | 110–164      | 7.052 69 | 1 489.99  | 203.57 |
| N-Methylacetamide         | 1   | 40–90        | 2.631 1  | 121.7     | –9.3   |
| Methyl acetate            | 1   | 1–56         | 7.065 2  | 1 157.63  | 219.73 |
| Methylal                  | 1   | 0–35         | 6.872 2  | 1 049.2   | 220.6  |
| Methylamine               | 1   | –83 to –6    | 7.336 9  | 1 011.5   | 233.3  |
| N-Methylaniline           | 1   | 50–200       | 7.081 9  | 1 631.3   | 192.4  |
| Methyl benzoate           | 1   | 111–199      | 7.273    | 1 847     | 221    |
| Methyl borate             | 1   | 31–68        | 7.646 0  | 1 491.5   | 245.5  |
| Methyl boric anhydride    | 1   | 0–55         | 8.004 1  | 1 726.1   | 257.9  |
| 2-Methyl-1,3-butadiene    | 1   | –52 to –24   | 7.011 87 | 1 126.159 | 238.88 |
|                           | 1   | –19 to 55    | 6.885 64 | 1 071.578 | 233.51 |
| 3-Methyl-1,2-butadiene    | 1   | –45 to –20   | 7.151 95 | 1 194.537 | 239.47 |
|                           | 1   | –20 to 62    | 6.943 50 | 1 103.901 | 230.89 |
| 2-Methylbutane            | 1   | –57 to 49    | 6.833 15 | 1 040.73  | 235.45 |
| 2-Methyl-1-butanethiol    | 1   | liq          | 6.913 85 | 1 347.317 | 215.07 |
| 3-Methyl-1-butanethiol    | 1   | liq          | 6.914 91 | 1 342.509 | 214.45 |
| 2-Methyl-2-butanethiol    | 1   | liq          | 6.828 37 | 1 254.885 | 218.76 |
| 2-Methyl-1-butanol        | 1   | 34–129       | 7.067 30 | 1 195.26  | 156.83 |
| 3-Methyl-1-butanol        | 1   | 25–153       | 7.258 21 | 1 314.36  | 169.36 |
| 2-Methyl-2-butanol        | 1   | 25–102       | 6.519 3  | 863.4     | 135.3  |
| 3-Methyl-2-butanol        | 1   | 25–111       | 6.942 1  | 1 090.9   | 157.2  |
| 2-Methyl-1-butene         | 1   | –53 to 52    | 6.846 37 | 1 039.69  | 236.65 |
| 3-Methyl-1-butene         | 1   | –63 to 41    | 6.824 55 | 1 012.37  | 236.65 |
| 2-Methyl-2-butene         | 1   | –48 to 60    | 6.966 59 | 1 124.33  | 236.63 |
| Methyl butyl ether        | 1   | 23–69        | 6.887 1  | 1 162.1   | 219.9  |
| 3-Methyl-1-butyne         | 1   | –55 to 47    | 6.884 80 | 1 014.81  | 227.11 |
| 2-Methyl-3-butyne-2-ol    | 1   | 21–106       | 6.657 5  | 976.5     | 154.1  |
| Methyl n-butyrate         | 1   |              | 6.972 11 | 1 272.73  | 208.5  |
| Methyl caprate            | 1   | 107–188      | 7.190 0  | 1 783.8   | 181.6  |
| Methyl caproate           | 1   | 44–105       | 7.409 3  | 1 672.74  | 218.98 |
| Methyl caprylate          | 1   | 100–146      | 6.916 5  | 1 496.3   | 176.5  |
| Methyl carbitol           | 1   | 112–193      | 7.424    | 1 751     | 192    |
| Methyl cellosolve acetate | 1   | 70–144       | 7.125 1  | 1 447.0   | 196.1  |
| Methyl chloroacetate      | 1   | 45–130       | 7.004 4  | 1 306.3   | 187.3  |
| Methylcyclohexane         | 1   | –3 to 127    | 6.823 00 | 1 270.763 | 221.42 |
| Methylcyclopentane        | 1   | –24 to 96    | 6.862 83 | 1 186.059 | 226.04 |
| Methyldichlorosilane      | 1   | 1–41         | 7.027 8  | 1 167.8   | 240.7  |
| 1-Methyl-2-ethylbenzene   | 1   | 48–194       | 7.003 14 | 1 535.374 | 207.30 |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                               | Eq. | Range, °C  | A        | B         | C       |
|-----------------------------------------|-----|------------|----------|-----------|---------|
| 1-Methyl-3-ethylbenzene                 | 1   | 46–190     | 7.015 82 | 1 529.184 | 208.51  |
| 1-Methyl-4-ethylbenzene                 | 1   | 46–191     | 6.998 02 | 1 527.113 | 208.92  |
| 1-Methyl-1-ethylcyclopentane            | 1   | 43–122     | 6.859 20 | 1 347.602 | 217.21  |
| 1-Methyl-2-ethylcyclopentane <i>cis</i> | 1   | 49–129     | 6.905 88 | 1 388.412 | 216.89  |
| 2-Methyl-3-ethylpentane                 | 1   |            | 6.867 31 | 1 318.12  | 215.31  |
| 3-Methyl-3-ethylpentane                 | 1   |            | 6.867 31 | 1 347     | 219.68  |
| 3-Methyl-5-ethylphenol                  | 1   | 111–233    | 7.958    | 2 236     | 208     |
| 2-Methyl-5-ethylpyridine                | 1   | 52–177     | 5.050    | 517       | 59      |
| <i>N</i> -Methylformamide               | 1   | 96–200     | 7.497 4  | 1 849.4   | 201.1   |
| Methyl formate                          | 1   | 21–32      | 3.027    | 3.02      | –11.9   |
| 2-Methylheptane                         | 1   | 42–119     | 6.917 35 | 1 337.47  | 213.69  |
| 3-Methylheptane                         | 1   | 43–120     | 6.899 44 | 1 331.53  | 212.41  |
| 4-Methylheptane                         | 1   |            | 6.900 65 | 1 327.66  | 212.57  |
| 2-Methylhexane                          | 1   | –9 to 115  | 6.873 18 | 1 236.026 | 219.55  |
| 3-Methylhexane                          | 1   | –8 to 117  | 6.867 64 | 1 240.196 | 219.22  |
| Methylhydrazine                         | 1   | 2–25       | 6.576 2  | 1 007.5   | 181.4   |
| <i>N</i> -Methylhydroxylamine           | 1   | 40–65      | 7.045 6  | 1 223.3   | 172.1   |
| <i>O</i> -Methylhydroxylamine           | 1   | –63 to 48  | 7.363 9  | 1 225.3   | 225.2   |
| Methyl isobutyl ketone                  | 1   | 22–116     | 6.672 7  | 1 168.4   | 191.9   |
| 1-Methyl-2-isopropylbenzene             | 1   | liq        | 6.940 4  | 1 548.05  | 203.15  |
| 1-Methyl-3-isopropylbenzene             | 1   | liq        | 6.940 5  | 1 539.05  | 203.93  |
| 1-Methyl-4-isopropylbenzene             | 1   | liq        | 6.923 7  | 1 537.06  | 203.05  |
| 3-Methylisoquinoline                    | 1   | 176–225    | 6.969 2  | 1 717.3   | 166.9   |
| Methyl isothiocyanate                   | 1   | 10–50      | 2.896 8  | 103.6     | 45.4    |
| Methyl laurate                          | 1   | 158–212    | 6.767 1  | 1 589.72  | 140.5   |
| Methyl linolate                         | 1   | 166–206    | 6.111 1  | 1 660.1   | 118.8   |
| Methyl methacrylate                     | 1   | 39–89      | 8.409 2  | 2 050.5   | 274.4   |
| Methyl myristate                        | 1   | 166–238    | 7.622 3  | 2 283.93  | 184.8   |
| 1-Methylnaphthalene                     | 1   | 108–278    | 7.035 92 | 1 826.948 | 195.00  |
| 2-Methylnaphthalene                     | 1   | 105–274    | 7.068 50 | 1 840.268 | 198.40  |
| Methyl oleate                           | 1   | 166–205    | 7.544 1  | 2 656.9   | 200.7   |
| Methyl palmitate                        | 1   | 148–202    | 9.594 4  | 4 146.43  | 297.76  |
| 2-Methylpentane                         | 1   | –32 to 83  | 6.839 10 | 1 135.410 | 226.57  |
| 3-Methylpentane                         | 1   | –30 to 87  | 6.848 87 | 1 152.368 | 227.13  |
| 2-Methyl-2-pentanethiol                 | 1   | 56–165     | 6.858 5  | 1 343.79  | 212.8   |
| 2-Methyl-1-pentanol                     | 1   | 25–150     | 7.520 1  | 1 564.7   | 189.2   |
| 2-Methyl-4-pentanol                     | 1   | 25–133     | 8.467 1  | 2 174.9   | 257.8   |
| 2-Methyl-1-pentene                      | 1   | –30 to 85  | 6.850 30 | 1 138.516 | 224.70  |
| 3-Methyl-1-pentene                      | 1   | –38 to 77  | 6.755 23 | 1 086.316 | 226.20  |
| 4-Methyl-1-pentene                      | 1   | –38 to 77  | 6.835 29 | 1 121.302 | 229.687 |
| 2-Methyl-2-pentene                      | 1   | –26 to 90  | 6.923 67 | 1 183.837 | 225.51  |
| 3-Methyl-2-pentene <i>cis</i>           | 1   | –26 to 91  | 6.910 73 | 1 186.402 | 226.70  |
| <i>trans</i>                            | 1   | –23 to 94  | 6.926 34 | 1 194.527 | 224.83  |
| 4-Methyl-2-pentene <i>cis</i>           | 1   | –35 to 79  | 6.841 29 | 1 120.707 | 226.59  |
| <i>trans</i>                            | 1   | –33 to 81  | 6.880 30 | 1 142.874 | 227.14  |
| Methyl phenyl ether                     | 1   | 110–164    | 7.052 69 | 1 489.99  | 203.57  |
| 2-Methylpiperidine                      | 1   | 51–158     | 6.818 59 | 1 274.61  | 205.40  |
| 2-Methylpropane                         | 1   | –87 to 7   | 6.910 48 | 946.35    | 246.68  |
| 2-Methyl-1-propanethiol                 | 1   | –10 to 113 | 6.887 46 | 1 237.282 | 220.31  |
| 2-Methyl-2-propanethiol                 | 1   | 1–88       | 6.787 81 | 1 115.565 | 221.31  |
| 2-Methyl-1-propanol                     | 1   | 20–115     | 7.327 05 | 1 248.48  | 172.92  |
| 2-Methyl-2-propanol                     | 1   | 26–83      | 9.170 6  | 2 206.4   | 267.9   |
| 2-Methylpropene                         | 1   | –82 to 12  | 6.684 66 | 866.25    | 234.64  |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                       | Eq. | Range, °C  | A        | B         | C      |
|---------------------------------|-----|------------|----------|-----------|--------|
| <i>N</i> -Methylpropionamide    | 1   | 30–90      | −0.9103  | 119.4     | −148.0 |
| Methyl propionate               | 1   | 21–79      | 6.942 4  | 1 170.2   | 208.8  |
| 2-Methyl-2-propylamine          | 1   | 19–75      | 6.783 2  | 993.33    | 210.50 |
| Methyl propyl ether             | 1   | 0–39       | 6.118 6  | 708.69    | 179.9  |
| 2-Methylpyridine                | 1   | 80–168     | 7.032 4  | 1 415.73  | 211.63 |
| 3-Methylpyridine                | 1   | 74–185     | 7.050 21 | 1 481.78  | 211.25 |
| 4-Methylpyridine                | 1   | 75–186     | 7.041 77 | 1 480.68  | 210.50 |
| 1-Methylpyrrole                 | 1   | 49–149     | 7.085 0  | 1 368.66  | 212.80 |
| 6-Methylquinoline               | 1   | 187–266    | 6.927 2  | 1 746.08  | 166.46 |
| 7-Methylquinoline               | 1   | 238–258    | 7.597 7  | 2 229.4   | 214.9  |
| Methyl salicylate               | 1   | 79–220     | 7.083 3  | 1 712.8   | 187.1  |
| Methyl stearate                 | 1   | 204–240    | 2.357 0  | 68.92     | −156.5 |
| <i>o</i> -Methylstyrene         | 1   | 32–112     | 7.212 9  | 1 664.08  | 214.59 |
| <i>m</i> -Methylstyrene         | 1   | 75–255     | 6.884 61 | 1 485.41  | 200.0  |
|                                 | 1   | 10–72      | 7.275 34 | 1 695.4   | 220.0  |
|                                 | 1   | 72–250     | 6.879 28 | 1 471.44  | 200.0  |
|                                 | 1   | 68–170     | 7.011 2  | 1 535.1   | 200.7  |
| <i>p</i> -Methylstyrene         | 1   | 68–170     | 7.011 2  | 1 535.1   | 200.7  |
| $\alpha$ -Methylstyrene         | 1   |            | 6.923 66 | 1 486.88  | 202.4  |
| $\beta$ -Methylstyrene          | 1   |            | 6.923 39 | 1 499.80  | 201.0  |
| Methyl sulfoxide                | 1   | 20–50      | 7.763 7  | 2 048.7   | 231.6  |
| 3-Methyl-2-thiabutane           | 1   | −13 to 109 | 6.901 96 | 1 232.170 | 221.67 |
| 2-Methylthiacyclopentane        | 1   | liq        | 6.944 12 | 1 409.503 | 214.41 |
| 3-Methylthiacyclopentane        | 1   | 67–179     | 6.949 1  | 1 431.8   | 213.6  |
| 2-Methyl-3-thiapentane          | 1   | liq        | 6.891 30 | 1 293.05  | 215.04 |
| Methyl-2-thiazole               | 1   | 80–128     | 7.042 1  | 1 407.05  | 209.33 |
| 2-Methylthiophene               | 1   | 9–138      | 6.938 97 | 1 326.48  | 214.31 |
| 3-Methylthiophene               | 1   | 11–141     | 6.986 11 | 1 363.83  | 216.78 |
| Methyl trichlorosilane          | 1   | 13–64      | 7.088 2  | 1 289.2   | 239.9  |
| 2-Methyl-5-vinylpyridine        | 1   | 69–183     | 6.156    | 1 023     | 129    |
| Morpholine                      | 1   | 0–44       | 7.718 13 | 1 745.8   | 235.0  |
| Naphthalene c                   | 1   | 44–170     | 7.160 30 | 1 447.70  | 210.0  |
|                                 | 1   | 86–250     | 7.010 65 | 1 733.71  | 201.86 |
| liq                             | 1   | 125–218    | 6.818 1  | 1 585.86  | 184.82 |
| 1-Naphthol                      | 1   | 141–282    | 7.284 21 | 2 077.56  | 184.0  |
| 2-Naphthol                      | 1   | 144–288    | 7.347 14 | 2 135.00  | 183.0  |
| Nicotine                        | 1   | 134–246    | 6.789    | 1 650     | 176    |
| <i>o</i> -Nitroaniline          | 2   | 150–260    | 8.868 4  | 3 336.50  |        |
| <i>m</i> -Nitroaniline          | 2   | 170–260    | 8.818 8  | 3 440.9   |        |
| <i>p</i> -Nitroaniline          | 2   | 190–260    | 9.559 5  | 4 039.73  |        |
| Nitrobenzene                    | 1   | 134–211    | 7.115 6  | 1 746.6   | 201.8  |
| <i>m</i> -Nitrobenzotrifluoride | 1   | 10–105     | 7.653 15 | 2 006.1   | 220.0  |
|                                 | 1   | 104–280    | 7.180 25 | 1 710.60  | 195.12 |
| Nitromethane                    | 1   | 56–136     | 7.281 66 | 1 446.94  | 227.60 |
| 1-Nitropropane                  | 1   | 59–131     | 7.114 6  | 1 467.45  | 215.23 |
| <i>o</i> -Nitrotoluene          | 1   | 129–222    | 5.851    | 946       | 96     |
| <i>p</i> -Nitrotoluene          | 1   | 148–233    | 6.994 8  | 1 720.39  | 184.9  |
| Nonadecane                      | 1   | 184–366    | 7.015 3  | 1 932.8   | 137.6  |
| 1-Nonadecene                    | 1   | liq        | 7.115 1  | 1 997.4   | 142.7  |
| Nonafluorocyclopentane          | 1   | 17–75      | 6.945 3  | 1 051.7   | 220.1  |
| Nonane                          | 1   | 39–179     | 6.938 93 | 1 431.82  | 202.01 |
| 1-Nonanethiol                   | 1   | 93–251     | 6.983 9  | 1 655.6   | 183.7  |
| Nonanoic acid                   | 1   | 137–177    | 3.235 9  | 143.97    | −75.6  |
| 1-Nonanol                       | 1   | 94–214     | 7.827 8  | 1 953.8   | 181.9  |



TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                                 | Eq. | Range, °C  | A        | B         | C       |
|-------------------------------------------|-----|------------|----------|-----------|---------|
| 1-Nonene                                  | 1   | 35–175     | 6.954 30 | 1 436.20  | 205.69  |
| Octadecane                                | 1   | 172–352    | 7.002 2  | 1 894.3   | 143.30  |
| 1-Octadecanethiol                         | 1   | liq        | 7.096    | 2 061     | 129     |
| 1-Octadecanol                             | 1   | 120–218    | 6.461 6  | 1 599     | 90      |
| 1-Octadecene                              | 1   |            | 7.060 65 | 1 997.4   | 147.50  |
| Octane                                    | 1   | 19–152     | 6.918 68 | 1 351.99  | 209.15  |
| 1-Octanethiol                             | 1   | 76–229     | 6.969 09 | 1 593.0   | 190.61  |
| 1-Octanol                                 | 1   | 0–80       | 12.070 1 | 4 506.8   | 319.9   |
|                                           | 1   | 70–195     | 6.837 90 | 1 310.62  | 136.05  |
| 2-Octanol                                 | 1   | 72–180     | 6.388 8  | 1 060.4   | 122.5   |
| 3-Octanol                                 | 1   | 76–176     | 5.221 5  | 560.3     | 64.7    |
| 4-Octanol                                 | 1   | 71–176     | 5.739 6  | 760.5     | 89.5    |
| 1-Octene                                  | 1   | 15–147     | 6.934 95 | 1 355.46  | 213.05  |
| 5-Oxyhydrindene                           | 1   | 120–251    | 9.213 7  | 3 665.8   | 326.4   |
| Pentachloroethane                         | 1   | 25–162     | 6.740    | 1 378     | 197     |
| Pentadecane                               | 1   | 136–304    | 7.023 59 | 1 789.95  | 161.38  |
| 1-Pentadecene                             | 1   |            | 7.022 91 | 1 788.58  | 163.347 |
| 1,2-Pentadiene                            | 1   | –42 to –26 | 7.259 90 | 1 250.293 | 241.96  |
|                                           | 1   | –21 to 67  | 6.918 20 | 1 104.991 | 228.85  |
| 1,3-Pentadiene <i>cis</i>                 | 1   | –43 to –22 | 7.193 87 | 1 223.602 | 240.62  |
|                                           | 1   | –18 to 66  | 6.910 89 | 1 101.923 | 229.37  |
| <i>trans</i>                              | 1   | –45 to –20 | 7.102 12 | 1 185.389 | 239.41  |
|                                           | 1   | –18 to 64  | 6.913 17 | 1 103.840 | 231.72  |
| 1,4-Pentadiene                            | 1   | –57 to –37 | 7.174 01 | 1 155.378 | 244.30  |
|                                           | 1   | –33 to 47  | 6.835 43 | 1 017.995 | 231.46  |
| 2,3-Pentadiene                            | 1   | –39 to –18 | 7.202 53 | 1 231.768 | 237.56  |
|                                           | 1   | –14 to 70  | 6.962 16 | 1 126.837 | 227.84  |
| Pentafluorobenzene                        | 1   | 49–94      | 7.036 65 | 1 254.07  | 216.02  |
| Pentafluorochloroacetone                  | 1   | –40 to 32  | 6.848 4  | 925.3     | 225.4   |
| Pentafluorochlorethane                    | 1   | –95 to –39 | 6.833 34 | 802.97    | 242.27  |
| Pentafluorophenol                         | 1   | 105–155    | 7.066 0  | 1 379.15  | 183.91  |
| 2,2,3,3,3-Pentafluoropropanol             | 1   | 0–23       | 6.308 7  | 830.56    | 153.8   |
| Pentafluorotoluene                        | 1   | 39–138     | 7.084 78 | 1 392.20  | 213.67  |
| <i>bis</i> -Pentamethyldisilanoxydisilane | 1   | 169–201    | 8.556 64 | 3 051.316 | 258.85  |
| <i>bis</i> -Pentamethyldisilanyl ether    | 1   | 88–183     | 8.161 44 | 2 575.250 | 273.32  |
| Pentane                                   | 1   | –50 to 58  | 6.852 96 | 1 064.84  | 233.01  |
| Pentanenitrile                            | 1   | 69–141     | 7.104 9  | 1 519.4   | 218.4   |
| 1-Pentanethiol                            | 1   | 19–153     | 6.933 11 | 1 369.479 | 211.31  |
| Pentanoic acid                            | 1   | 72–174     | 5.412    | 591       | 60      |
| 1-Pentanol                                | 1   | 37–138     | 7.177 58 | 1 314.56  | 168.11  |
| 2-Pentanol                                | 1   | 25–120     | 7.275 75 | 1 271.92  | 170.37  |
| 3-Pentanol                                | 1   | 21–116     | 7.414 93 | 1 354.42  | 183.41  |
| 2-Pentanone                               | 1   | 56–111     | 7.021 93 | 1 313.85  | 215.01  |
| 3-Pentanone                               | 1   | 56–111     | 7.025 29 | 1 310.28  | 214.19  |
| 1-Pentene                                 | 1   | –55 to 51  | 6.844 24 | 1 044.01  | 233.50  |
| 2-Pentene <i>cis</i>                      | 1   | –49 to 58  | 6.843 08 | 1 052.44  | 228.69  |
| <i>trans</i>                              | 1   | –49 to 58  | 6.899 83 | 1 080.76  | 232.57  |
| 1-Pentyne                                 | 1   | –44 to 61  | 6.967 34 | 1 092.52  | 227.18  |
| 2-Pentyne                                 | 1   | –33 to 78  | 7.046 14 | 1 189.87  | 229.60  |
| Perdeuterobenzene                         | 1   | 10–82      | 6.892 35 | 1 198.39  | 219.43  |
| Perdeuterocyclohexane                     | 1   | 10–80      | 6.837 86 | 1 190.38  | 222.40  |
| Perfluorobutane                           | 1   | –39 to –4  | 7.035 1  | 990.27    | 240.4   |
| Perfluorobutene                           | 1   | –28 to 20  | 9.222    | 2 401.6   | 382     |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                     | Eq. | Range, °C   | A        | B         | C      |
|-------------------------------|-----|-------------|----------|-----------|--------|
| Perfluorocyclobutane          | 1   | −32 to 0    | 6.815 29 | 862.49    | 225.19 |
| Perfluorocyclohexane          | 1   | 19–65       | 6.04     | 597       | 136    |
| Perfluorocyclopentane         | 1   | 17–56       | 7.039 6  | 1 069.3   | 234.6  |
| Perfluoroheptane              | 1   | −2 to 106   | 6.937 72 | 1 181.14  | 208.66 |
| Perfluorohexane               | 1   | 30–57       | 6.875 2  | 1 080.8   | 213.4  |
| Perfluoromethylcyclohexane    | 1   | 33–111      | 6.824 06 | 1 133.76  | 211.22 |
| Perfluorooctane               | 1   | 37–105      | 5.902 5  | 1 225.93  | 198.99 |
| Perfluoropentane              | 1   | 9–65        | 7.017 9  | 1 072.9   | 230.0  |
| Perfluoropiperidine           | 1   | 29–81       | 6.853 4  | 1 059.95  | 217.2  |
| Perfluoropropane              | 1   | −79 to −36  | 6.919 4  | 825.8     | 241.2  |
| Perfluoropropene              | 1   | −41 to 20   | 7.355    | 1 012.1   | 257    |
| Phenanthrene                  | 1   | 176–379     | 7.260 82 | 2 379.04  | 203.76 |
| Phenol                        | 1   | 107–182     | 7.133 0  | 1 516.79  | 174.95 |
| $\beta$ -Phenylethyl acetate  | 1   | 149–233     | 6.834 3  | 1 555.2   | 160.8  |
| $\alpha$ -Phenylethyl alcohol | 1   | 82–190      | 1.508    | 91        | −263   |
| <i>o</i> -Phenylethylphenol   | 1   | 169–250     | 4.506 0  | 516.8     | −32.1  |
| <i>p</i> -Phenylethylphenol   | 1   | 174–251     | 4.304 1  | 459.3     | −52.4  |
| Phenylisocyanate              | 1   | 10–80       | −0.708 0 | 106.4     | −146.6 |
| 4-Phenylphenol                | 1   | 177–308     | 8.657 5  | 3 022.8   | 216.1  |
| Phosgene                      | 1   | −68 to 68   | 6.842 97 | 941.25    | 230    |
| Phthalic anhydride            | 2   | 160–285     | 8.022    | 2 868.5   |        |
| $\alpha$ -Pinene              | 1   | 19–156      | 6.852 5  | 1 446.4   | 208.0  |
| $\beta$ -Pinene               | 1   | 19–166      | 6.898 4  | 1 511.7   | 210.2  |
| Piperidine                    | 1   | 42–144      | 6.855 69 | 1 238.80  | 205.43 |
| Propadiene                    | 1   | −99 to −16  | 5.713 7  | 458.06    | 196.07 |
| Propane                       | 1   | −108 to −25 | 6.803 38 | 804.00    | 247.04 |
| 1-Propanethiol                | 1   | −25 to 91   | 6.928 46 | 1 183.307 | 224.62 |
| 2-Propanethiol                | 1   | −37 to 75   | 6.877 34 | 1 113.895 | 226.16 |
| 1-Propanol                    | 1   | 2–120       | 7.847 67 | 1 499.21  | 204.64 |
| 2-Propanol                    | 1   | 0–101       | 8.117 78 | 1 580.92  | 219.61 |
| 2-Propen-1-ol                 | 1   | 21–97       | 11.187 0 | 4 068.5   | 392.7  |
| Propionic acid                | 1   | 56–139.5    | 6.403    | 950.2     | 130.3  |
| Propionic anhydride           | 1   | 67–167      | 5.819 5  | 810.3     | 108.7  |
| Propionitrile                 | 1   | −84 to 22   | 5.278 2  | 665.52    | 159.10 |
| Propiophenone                 | 1   | 132–201     | 7.370    | 1 894     | 205    |
| Propyl acetate                | 1   | 39–101      | 7.016 15 | 1 282.28  | 208.60 |
| 1-Propylamine                 | 1   | 23–77       | 6.926 51 | 1 044.05  | 210.84 |
| 2-Propylamine                 | 1   | 4–61        | 6.890 25 | 985.69    | 214.07 |
| <i>n</i> -Propylbenzene       | 1   | 43–188      | 6.951 42 | 1 491.297 | 207.14 |
| <i>n</i> -Propyl borate       | 1   | 85–179      | 7.399 8  | 1 741     | 206    |
| <i>n</i> -Propyl caprate      | 1   | 97–186      | 8.701 22 | 2 945.99  | 253.63 |
| <i>n</i> -Propyl caproate     | 1   | 43–120      | 8.667 1  | 2 556.0   | 262.9  |
| <i>n</i> -Propyl caprylate    | 1   | 70–153      | 8.516 7  | 2 599.5   | 246.2  |
| <i>n</i> -Propyl cellosolve   | 1   | 77–149      | 7.146 4  | 1 440.6   | 187.7  |
| <i>n</i> -Propylcyclohexane   | 1   | 40–186      | 6.886 46 | 1 460.800 | 207.94 |
| <i>n</i> -Propylcyclopentane  | 1   | 21–158      | 6.903 92 | 1 384.386 | 213.16 |
| Propylene                     | 1   | −112 to −32 | 6.778 11 | 770.85    | 245.51 |
| 1,2-Propylene oxide           | 1   | −35 to 130  | 7.064 92 | 1 113.6   | 232    |
| <i>n</i> -Propyl formate      | 1   | 26–82       | 6.848    | 1 127     | 203    |
| <i>n</i> -Propyl laurate      | 1   | 124–205     | 8.068 9  | 2 692.4   | 222.5  |
| <i>n</i> -Propyl myristate    | 1   | 147–200     | 9.216 8  | 3 744.68  | 272.87 |
| <i>n</i> -Propyl nitrate      | 1   | 0–70        | 6.954 9  | 1 294.4   | 206.7  |
| <i>n</i> -Propyl palmitate    | 1   | 166–204     | 14.129 2 | 9 759.2   | 539.7  |

TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                               | Eq. | Range, °C   | A        | B         | C      |
|-----------------------------------------|-----|-------------|----------|-----------|--------|
| <i>o</i> -( <i>n</i> -Propyl)phenol     | 1   | 104–222     | 9.215    | 3 254     | 292    |
| <i>p</i> -( <i>n</i> -Propyl)phenol     | 1   | 0–234       | 8.329 6  | 2 661     | 254    |
| <i>n</i> -Propyl phenyl ether           | 1   | 101–190     | 7.734 3  | 2 146.2   | 252.3  |
| Propyne                                 | 1   | –90 to –6   | 6.784 85 | 803.73    | 229.08 |
| Pseudocumenol                           | 1   | 107–232     | 6.915    | 1 547     | 152    |
| Pyrene                                  | 1   | 200–395     | 5.618 4  | 1 122.0   | 15.2   |
| Pyridine                                | 1   | 67–153      | 7.041 15 | 1 373.80  | 214.98 |
| Pyrogallol                              | 1   | 177–309     | 6.092    | 1 031     | 12     |
| Pyrrole                                 | 1   | 66–166      | 7.294 70 | 1 501.56  | 210.42 |
| Quinaldine                              | 1   | 178–248     | 7.179 00 | 1 857.84  | 184.50 |
| Quinoline                               | 1   | 164–238     | 6.817 59 | 1 668.73  | 186.26 |
| Spiropentane                            | 1   | 3–71        | 6.917 00 | 1 090.08  | 231.10 |
| Styrene                                 | 1   | 32–82       | 7.140 16 | 1 574.51  | 224.09 |
| Terpenyl acetate                        | 1   | 37–150      | 6.443 46 | 1 377.27  | 143.85 |
| $\alpha$ -Terpineol                     | 1   | 84–217      | 8.141 2  | 2 479.4   | 253.7  |
| Terpinolene                             | 1   | 40–179      | 7.169    | 1 706     | 211    |
| Tetrabutyl tin                          | 1   | 100–300     | 6.545    | 1 649     | 148    |
| 1,1,2,2-Tetrachloro-1,2-difluoro-ethane | 1   | 10–91.5     | 10.995   | 4 437.1   | 455.2  |
| 1,1,1,2-Tetrachloroethane               | 1   | 59–130      | 6.898 75 | 1 365.88  | 209.74 |
| 1,1,2,2-Tetrachloroethane               | 1   | 25–130      | 6.631 7  | 1 228.1   | 179.9  |
| Tetrachloroethylene                     | 1   | 37–120      | 6.976 83 | 1 386.92  | 217.53 |
| Tetrachloromethane                      | 1   |             | 6.879 26 | 1 212.021 | 226.41 |
| Tetradecane                             | 1   | 122–286     | 7.013 00 | 1 740.88  | 167.72 |
| 1-Tetradecanethiol                      | 1   |             | 7.048 5  | 1 909.2   | 151.9  |
| 1-Tetradecanol                          | 1   | 130–264     | 6.674 1  | 1 204.5   | 54.0   |
| 1-Tetradecene                           | 1   | 119–283     | 7.030 65 | 1 754.09  | 171.52 |
| 1,2,3,4-Tetrafluorobenzene              | 1   | 6–50        | 7.084 6  | 1 339.23  | 223.49 |
| 1,2,3,5-Tetrafluorobenzene              | 1   | 6–50        | 6.986 17 | 1 245.20  | 218.35 |
| Tetrafluoroethylene                     | 1   | –131 to –65 | 6.896 59 | 683.84    | 245.93 |
| Tetrafluoromethane                      | 1   |             | 6.972 31 | 540.50    | 260.10 |
| Tetrahydrofuran                         | 1   | 23–100      | 6.995 15 | 1 202.29  | 226.25 |
| Tetraiodothiophene                      | 1   | –65 to 24   | 5.585 44 | 871.25    | 175.59 |
| Tetralin                                | 1   | 94–206      | 7.070 55 | 1 741.30  | 208.26 |
| 1,2,3,4-Tetramethylbenzene              | 1   | 80–217      | 7.059 4  | 1 690.54  | 199.48 |
| 1,2,3,5-Tetramethylbenzene              | 1   | 75–228      | 7.077 9  | 1 675.43  | 201.14 |
| 1,2,4,5-Tetramethylbenzene              | 1   | 74–227      | 7.080 0  | 1 672.43  | 201.43 |
| 2,2,3,3-Tetramethylbutane               | 1   | 0–65        | 6.876 65 | 1 329.93  | 226.36 |
| Tetramethyl lead                        | 1   | 0–60        | 6.937 7  | 1 335.3   | 219.1  |
| 2,2,3,3-Tetramethylpentane              | 1   | 57–141      | 6.830 60 | 1 398.67  | 213.84 |
| 2,2,3,4-Tetramethylpentane              | 1   | 52–134      | 6.834 18 | 1 375.59  | 214.94 |
| 2,2,4,4-Tetramethylpentane              | 1   | 43–123      | 6.796 20 | 1 324.59  | 216.02 |
| Tetramethylsilane                       | 1   | –64 to 21   | 6.822 39 | 1 033.72  | 235.62 |
| 2-Thiabutane                            | 1   | –26 to 90   | 6.938 49 | 1 182.562 | 224.78 |
| Thiacyclobutane                         | 1   | –5 to 120   | 7.016 67 | 1 321.331 | 224.51 |
| Thiacyclohexane                         | 1   | 29–170      | 6.905 18 | 1 422.47  | 211.72 |
| Thiacyclopentane                        | 1   | 14–148      | 6.995 40 | 1 401.939 | 219.61 |
| Thiacyclopropane                        | 1   | –35 to 77   | 7.037 25 | 1 194.37  | 232.42 |
| 3-Thiaheptane                           | 1   | 33–172      | 6.941 02 | 1 421.32  | 205.81 |
| 4-Thiaheptane                           | 1   | 32–170      | 6.935 77 | 1 413.44  | 205.73 |
| 2-Thiahexane                            | 1   | 17–150      | 6.945 83 | 1 363.808 | 212.07 |
| 3-Thiahexane                            | 1   | 14–144      | 6.933 80 | 1 341.57  | 212.51 |

**TABLE 5.9** Vapor Pressures of Various Organic Compounds (*Continued*)

| Substance                                     | Eq. | Range, °C   | A        | B         | C      |
|-----------------------------------------------|-----|-------------|----------|-----------|--------|
| 2-Thiapentane                                 | 1   | −4 to 120   | 6.955 45 | 1 284.32  | 219.66 |
| 3-Thiapentane                                 | 1   | −13 to 109  | 6.928 36 | 1 257.833 | 218.66 |
| 2-Thiapropane                                 | 1   | −47 to 58   | 6.948 79 | 1 090.755 | 230.80 |
| Thiazole                                      | 1   | 63–118      | 7.142 01 | 1 425.35  | 216.26 |
| Thiophene                                     | 1   | −12 to 108  | 6.959 26 | 1 246.02  | 221.35 |
| Toluene                                       | 1   | 6–137       | 6.954 64 | 1 344.800 | 219.48 |
| <i>o</i> -Toluidine                           | 1   | 118–200     | 7.082 03 | 1 627.72  | 187.13 |
| <i>m</i> -Toluidine                           | 1   | 122–203     | 7.093 67 | 1 631.43  | 183.91 |
| <i>p</i> -Toluidine                           | 1   |             | 7.260 22 | 1 758.55  | 201.0  |
| <i>m</i> -Tolyl pentafluoropropionate         | 1   | 98–174      | 7.427 20 | 1 707.59  | 201.70 |
| <i>p</i> -Tolyl pentafluoropropionate         | 1   | 99–176      | 8.078 6  | 2 223.8   | 252.1  |
| <i>m</i> -Tolyl trifluoroacetate              | 1   | 91–166      | 7.681 0  | 1 874.84  | 223.48 |
| <i>p</i> -Tolyl trifluoroacetate              | 1   | 92–169      | 7.913 8  | 2 055.41  | 238.99 |
| Tribromomethane                               | 1   | 30–101      | 6.821 8  | 1 376.7   | 201.0  |
| 1,2,3-Tribromopropane                         | 1   | 128–205     | 7.037 2  | 1 735.32  | 195.42 |
| Trichloroacetic acid                          | 1   | 112–198     | 7.273 0  | 1 594.3   | 165.4  |
| Trichloroacetonitrile                         | 1   | 17–83       | 7.183 5  | 1 368.3   | 232.5  |
| Trichloroacetyl chloride                      | 1   | 32–119      | 6.990 75 | 1 390.47  | 220.11 |
| 1,1,1-Trichloroethane                         | 1   | −6 to 17    | 8.643 4  | 2 136.6   | 302.8  |
| 1,1,2-Trichloroethane                         | 1   | 50–114      | 6.951 85 | 1 314.41  | 209.20 |
| Trichloroethylene                             | 1   | 18–86       | 6.518 3  | 1 018.6   | 192.7  |
| Trichlorofluoromethane                        | 1   |             | 6.884 28 | 1 043.004 | 236.88 |
| Trichlorosilane                               | 1   | 2–32        | 6.773 9  | 1 009.0   | 227.2  |
| <i>bis</i> -(Trichlorosilyl)ethane            | 1   | 91–160      | 7.835 11 | 2 241.769 | 249.84 |
| 1,1,1-Trichloro-2,2,2-trifluoroethane         | 1   | 14–36       | 4.437 3  | 204.1     | 83.9   |
| 1,1,2-Trichloro-1,2,2-trifluoroethane         | 1   | −25 to 83   | 6.880 3  | 1 099.9   | 227.5  |
| Tridecane                                     | 1   | 107–267     | 7.007 56 | 1 690.67  | 174.22 |
| 1-Tridecene                                   | 1   | 105–264     | 6.981 02 | 1 672.00  | 174.95 |
| Triethanolamine                               | 1   | 252–305     | 10.067 5 | 4 542.78  | 297.76 |
| Triethyl aluminum                             | 1   | 57–126      | 11.646 1 | 4 466.59  | 322.87 |
| Triethylamine                                 | 1   | 50–95       | 5.858 8  | 695.7     | 144.8  |
| Triethyl borate                               | 1   | 29–109      | 7.511 1  | 1 641.7   | 236.3  |
| Triethylsilanol                               | 1   | 24–140      | 7.793 7  | 1 756.1   | 202.4  |
| Trifluoroacetic acid                          | 1   | 12–72       | 8.389    | 1 895     | 273    |
| Trifluoroacetic anhydride                     | 1   | −2 to 39    | 6.135 8  | 1 026.1   | 202.0  |
| Trifluoroacetonitrile                         | 1   | −132 to −68 | 7.127 6  | 773.82    | 249.9  |
| 1,3,5-Trifluorobenzene                        | 1   | 6–50        | 6.919 8  | 1 197.13  | 219.12 |
| Trifluorochloroethylene                       | 1   | −67 to −11  | 6.896 16 | 848.33    | 293.64 |
| 1,1,1-Trifluoroethane                         | 1   | −110 to −48 | 6.903 78 | 788.20    | 243.23 |
| 2,2,2-Trifluoroethanol                        | 1   | −0.5 to 25  | 6.788 2  | 978.13    | 173.06 |
| Trifluoromethane                              | 1   | −128 to −82 | 7.088 6  | 705.33    | 249.78 |
| <i>bis</i> -(Trifluoromethyl)-acetoxyporphine | 1   | 0–40        | 7.391 31 | 1 426.254 | 220.37 |
| 2,2,2-Trifluoro-1-methylbenzene               | 1   | 55–139      | 6.970 45 | 1 306.35  | 217.38 |
| <i>bis</i> -(Trifluoromethyl)-chlorophosphine | 1   | −80 to 0    | 7.661 06 | 1 386.652 | 267.14 |
| Trifluoromethylhypofluorite                   | 1   | 145–189     | 6.950 6  | 650.1     | −18.4  |
| <i>bis</i> -(Trifluoromethyl)-iodophosphine   | 1   | 0–47        | 6.901 39 | 1 180.723 | 222.95 |
| Triisobutylene                                | 1   | 56–179      | 7.002 1  | 1 613.47  | 212.5  |

TABLE 5.9 Vapor Pressures of Various Organic Compounds (Continued)

| Substance                      | Eq. | Range, °C  | A        | B         | C      |
|--------------------------------|-----|------------|----------|-----------|--------|
| Trimethyl aluminum             | 1   | 64–127     | 7.570 29 | 1 734.72  | 242.78 |
| Trimethylamine                 | 1   | –80 to 3   | 6.857 55 | 955.94    | 237.52 |
| 1,2,3-Trimethylbenzene         | 1   | 57–205     | 7.040 82 | 1 593.958 | 207.08 |
| 1,2,4-Trimethylbenzene         | 1   | 52–198     | 7.043 83 | 1 573.257 | 208.56 |
| 1,3,5-Trimethylbenzene         | 1   | 49–193     | 7.074 36 | 1 569.622 | 209.58 |
| 2,2,3-Trimethylbutane          | 1   | –19 to 106 | 6.792 30 | 1 200.563 | 226.05 |
| Trimethylchlorosilane          | 1   | 2–55       | 7.055 8  | 1 245.5   | 240.7  |
| 1,1,3-Trimethylcyclohexane     | 1   | 55–137     | 6.839 51 | 1 394.88  | 215.73 |
| 1,1,2-Trimethylcyclopentane    | 1   | 36–115     | 6.822 38 | 1 309.81  | 218.58 |
| 1,1,3-Trimethylcyclopentane    | 1   | 29–106     | 6.809 31 | 1 275.92  | 219.89 |
| 1,2,4-Trimethylcyclopentane    |     |            |          |           |        |
| <i>cis, cis, trans</i>         | 1   | 39–118     | 6.857 38 | 1 335.69  | 219.16 |
| <i>cis, trans, cis</i>         | 1   | 33–110     | 6.851 3  | 1 307.10  | 219.92 |
| 1,3,5-Trimethyl-2-ethylbenzene | 1   | 88–210     | 6.790 8  | 1 505.8   | 174.7  |
| 1,4,5-Trimethyl-2-ethylbenzene | 1   | 87–132     | 3.029 3  | 116.4     | –34.6  |
| 2,2,5-Trimethylhexane          | 1   | 46–125     | 6.837 75 | 1 325.54  | 210.91 |
| 2,4,4-Trimethylhexane          | 1   | 51–131     | 6.856 54 | 1 371.81  | 214.40 |
| Trimethylhydrazine             | 1   | –16 to 14  | 7.106 80 | 1 189.88  | 222.06 |
| O,N,N-Trimethylhydroxylamine   | 1   | –79 to 23  | 6.765 8  | 979.55    | 222.2  |
| 2,2,3-Trimethylpentane         | 1   |            | 6.825 46 | 1 294.88  | 218.42 |
| 2,2,4-Trimethylpentane         | 1   | 24–100     | 6.811 89 | 1 257.84  | 220.74 |
| 2,3,3-Trimethylpentane         | 1   |            | 6.843 53 | 1 328.05  | 220.38 |
| 2,3,4-Trimethylpentane         | 1   | 36–114     | 6.853 96 | 1 315.08  | 217.53 |
| 2,4,4-Trimethyl-1-pentene      | 1   | –3 to 128  | 6.834 57 | 1 273.416 | 220.62 |
| 2,4,4-Trimethyl-2-pentene      | 1   | 2–131      | 6.859 22 | 1 272.717 | 214.99 |
| 2,3,5-Trimethylphenol          | 1   | 186–247    | 7.080 12 | 1 685.90  | 166.14 |
| Trimethylsilanol               | 1   | 18–85      | 8.126 6  | 1 657.6   | 219.2  |
| 2,4,5-Trimethylstyrene         | 1   | 79–216     | 7.331 5  | 1 880.7   | 205.7  |
| 2,4,6-Trimethylstyrene         | 1   | 90–208     | 7.089 1  | 1 702.61  | 195.93 |
| 1,2,4-Trinitrobenzene          | 1   | 250–300    | 3.194    | 87        | –199   |
| 1,3,5-Trinitrobenzene          | 1   | 202–312    | 5.534 5  | 993.6     | 11.2   |
| 2,4,6-Trinitrobenzene          | 1   | 249–342    | 9.621 1  | 4 987.9   | 329.9  |
| 2,4,6-Trinitrotoluene          | 1   | 230–250    | 7.671 52 | 2 669.4   | 205.6  |
| α-Trioxane                     | 1   | 56–114     | 7.818 6  | 1 783.3   | 247.1  |
| Trivinylarsine                 | 1   | 22–66      | 7.894 1  | 2 115.6   | 293.9  |
| Trivinyl bismuth               | 1   | 20–74      | 7.237 2  | 1 667.0   | 215.1  |
| Trivinylphosphine              | 1   | 16–61      | 7.928 4  | 2 102.0   | 301.3  |
| Trivinylstibine                | 1   | 20–70      | 8.322 1  | 2 446.3   | 303.8  |
| Undecane                       | 1   | 75–226     | 6.972 20 | 1 569.57  | 187.70 |
| 1-Undecanethiol                | 1   |            | 7.012 2  | 1 767.4   | 170.4  |
| 1-Undecene                     | 1   | 72–222     | 6.966 77 | 1 563.21  | 189.87 |
| Urethane                       | 1   |            | 7.421 64 | 1 758.21  | 205.0  |
| Vinyl acetate                  | 1   | 22–72      | 7.210 1  | 1 296.13  | 226.66 |
| o-Xylene                       | 1   | 32–172     | 6.998 91 | 1 474.679 | 213.69 |
| m-Xylene                       | 1   | 28–166     | 7.009 08 | 1 462.266 | 215.11 |
| p-Xylene                       | 1   | 27–166     | 6.990 52 | 1 453.430 | 215.31 |
| 2,3-Xylenol                    | 1   | 149–218    | 7.053 97 | 1 617.57  | 170.74 |
| 2,4-Xylenol                    | 1   | 144–212    | 7.055 39 | 1 587.46  | 169.34 |
| 2,5-Xylenol                    | 1   | 144–212    | 7.051 56 | 1 592.70  | 170.74 |
| 2,6-Xylenol                    | 1   | 145–204    | 7.070 70 | 1 628.32  | 187.60 |
| 3,4-Xylenol                    | 1   | 172–229    | 7.079 19 | 1 621.45  | 159.26 |
| 3,5-Xylenol                    | 1   | 155–223    | 7.130 76 | 1 639.86  | 164.16 |

5.3 BOILING POINTS

TABLE 5.10 Boiling Points of Water

| A. Barometric Pressures at Various Temperatures |          |          |          |          |          |
|-------------------------------------------------|----------|----------|----------|----------|----------|
| Temp. °C.                                       | 0.0°     | 0.2°     | 0.4°     | 0.6°     | 0.8°     |
|                                                 | mm of Hg | mm of Hg | mm of Hg | mm of Hg | mm of Hg |
| 80                                              | 355.40   | 358.28   | 361.19   | 364.11   | 367.06   |
| 81                                              | 370.03   | 373.01   | 376.02   | 379.05   | 382.09   |
| 82                                              | 385.16   | 388.25   | 391.36   | 394.49   | 397.64   |
| 83                                              | 400.81   | 404.00   | 407.22   | 410.45   | 413.71   |
| 84                                              | 416.99   | 420.29   | 423.61   | 426.95   | 430.32   |
| 85                                              | 433.71   | 437.12   | 440.55   | 444.01   | 447.49   |
| 86                                              | 450.99   | 454.51   | 458.06   | 461.63   | 465.22   |
| 87                                              | 468.84   | 472.48   | 476.14   | 479.83   | 483.54   |
| 88                                              | 487.28   | 491.04   | 494.82   | 498.63   | 502.46   |
| 89                                              | 506.32   | 510.20   | 514.11   | 518.04   | 521.99   |
| 90                                              | 525.97   | 529.98   | 534.01   | 538.07   | 542.15   |
| 91                                              | 546.26   | 550.40   | 554.56   | 558.75   | 562.96   |
| 92                                              | 567.20   | 571.47   | 575.76   | 580.08   | 584.43   |
| 93                                              | 588.80   | 593.20   | 597.63   | 602.09   | 606.57   |
| 94                                              | 611.08   | 615.62   | 620.19   | 624.79   | 629.41   |
| 95                                              | 634.06   | 638.74   | 643.45   | 648.19   | 652.96   |
| 96                                              | 657.75   | 662.58   | 667.43   | 672.32   | 677.23   |
| 97                                              | 682.18   | 687.15   | 692.15   | 697.19   | 702.25   |
| 98                                              | 707.35   | 712.47   | 717.63   | 722.81   | 728.03   |
| 99                                              | 733.28   | 738.56   | 743.87   | 749.22   | 754.59   |
| 100                                             | 760.00   | 765.44   | 770.91   | 776.42   | 781.95   |

| B. Boiling Points of Water at Various Pressures |                    |                |                    |                |                    |                |                    |
|-------------------------------------------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| Pressure, atm.                                  | Boiling Point, °C. | Pressure, atm. | Boiling Point, °C. | Pressure, atm. | Boiling Point, °C. | Pressure, atm. | Boiling Point, °C. |
| 0.5                                             | 80.9               | 7              | 164.2              | 14             | 194.1              | 21             | 213.9              |
| 1                                               | 100.0              | 8              | 169.6              | 15             | 197.4              | 22             | 216.2              |
| 2                                               | 119.6              | 9              | 174.5              | 16             | 200.4              | 23             | 218.5              |
| 3                                               | 132.9              | 10             | 179.0              | 17             | 203.4              | 24             | 220.8              |
| 4                                               | 142.9              | 11             | 183.2              | 18             | 206.1              | 25             | 222.9              |
| 5                                               | 151.1              | 12             | 187.1              | 19             | 208.8              | 26             | 225.0              |
| 6                                               | 158.1              | 13             | 190.7              | 20             | 211.4              | 27             | 227.0              |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures  
*An azeotrope is a mixture that cannot be separated by distillation.*

| A. Binary azeotropes containing water |                        |                   |                 |
|---------------------------------------|------------------------|-------------------|-----------------|
| System                                | BP of azeotrope,<br>°C | Composition, wt % |                 |
|                                       |                        | Water             | Other component |
| Inorganic acids                       |                        |                   |                 |
| Hydrogen bromide                      | 126                    | 52.5              | 47.5            |
| Hydrogen chloride                     | 108.58                 | 79.78             | 20.22           |
| Hydrogen fluoride                     | 111.35                 | 64.4              | 35.6            |
| Hydrogen iodide                       | 127                    | 43                | 57              |
| Hydrogen peroxide                     | zeotrope               |                   |                 |
| Nitric acid                           | 120.7                  | 32.6              | 67.4            |
| Perchloric acid                       | 203                    | 28.4              | 71.6            |
| Organic acids                         |                        |                   |                 |
| Formic acid                           | 107.2                  | 22.6              | 77.4            |
| Acetic acid                           | zeotrope               |                   |                 |
| Propionic acid                        | 99.9                   | 82.3              | 17.7            |
| Isobutyric acid                       | 99.3                   | 79                | 21              |
| Butyric acid                          | 99.4                   | 81.6              | 18.4            |
| Pentanoic acid                        | 99.8                   | 89                | 11              |
| Isopentanoic acid                     | 99.5                   | 81.6              | 18.4            |
| Perfluorobutyric acid                 | 97                     | 71                | 29              |
| Crotonic acid                         | 99.9                   | 97.8              | 2.2             |
| Alcohols                              |                        |                   |                 |
| Ethanol                               | 78.17                  | 4                 | 96              |
| Allyl alcohol                         | 88.9                   | 27.7              | 72.3            |
| 1-Propanol                            | 71.7                   | 71.7              | 28.3            |
| 2-Propanol                            | 80.3                   | 12.6              | 87.4            |
| 1-Butanol                             | 92.7                   | 42.5              | 57.5            |
| 2-Butanol                             | 87.0                   | 26.8              | 73.2            |
| 2-Methyl-2-propanol                   | 79.9                   | 11.7              | 88.3            |
| 1-Pentanol                            | 95.8                   | 54.4              | 45.6            |
| 2-Pentanol                            | 91.7                   | 36.5              | 63.5            |
| 3-Pentanol                            | 91.7                   | 36.0              | 64.0            |
| 2,2-Dimethyl-2-propanol               | 87.35                  | 27.5              | 72.5            |
| 1-Hexanol                             | 97.8                   | 67.2              | 32.8            |
| 1-Octanol                             | 99.4                   | 90                | 10              |
| Cyclopentanol                         | 96.25                  | 58                | 42              |
| 1-Heptanol                            | 98.7                   | 83                | 17              |
| Phenol                                | 99.52                  | 90.8              | 9.2             |
| 2-Methoxyphenol                       | 99.5                   | 87.5              | 12.5            |
| 1-Phenylphenol                        | 99.95                  | 98.75             | 1.25            |
| Benzyl alcohol                        | 99.9                   | 91                | 9               |
| 2,3-Dimethyl-2,3-butanediol           | zeotrope               |                   |                 |
| Furfuryl alcohol                      | 98.5                   | 80                | 20              |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                            | BP of azeotrope,<br>°C | Composition, wt % |                    |
|-----------------------------------|------------------------|-------------------|--------------------|
|                                   |                        | Water             | Other<br>component |
| Aldehydes                         |                        |                   |                    |
| Propionaldehyde                   | 47.5                   | 2                 | 98                 |
| Butyraldehyde                     | 68                     | 6                 | 94                 |
| Pentanal                          | 83                     | 19                | 81                 |
| Paraldehyde                       | 90                     | 28.5              | 71.5               |
| Furaldehyde                       | 97.5                   | 65                | 35                 |
| Amines                            |                        |                   |                    |
| <i>N</i> -Methylbutylamine        | 82.7                   | 15                | 85                 |
| Furfurylamine                     | 99                     | 74                | 26                 |
| Piperidine                        | 92.8                   | 35                | 65                 |
| Pyridine                          | 93.6                   | 41.3              | 58.7               |
| 2-Methylpyridine                  | 93.5                   | 48                | 52                 |
| 3-Methylpyridine                  | 97                     | 60                | 40                 |
| 4-Methylpyridine                  | 97.35                  | 62.8              | 37.2               |
| 2,6-Dimethylpyridine              | 96.02                  | 51.8              | 48.2               |
| Dibutylamine                      | 97                     | 50.5              | 49.5               |
| Dihexylamine                      | 99.8                   | 92.8              | 7.2                |
| Triallylamine                     | 95                     | 38                | 62                 |
| Tributylamine                     | 99.65                  | 79.7              | 20.3               |
| Aniline                           | 98.6                   | 80.8              | 19.2               |
| <i>N</i> -Ethylaniline            | 99.2                   | 83.9              | 16.1               |
| 1-Methyl-2-(2-pyridyl)pyrrolidine | 99.85                  | 97.5              | 2.5                |
| Halogenated hydrocarbons          |                        |                   |                    |
| Chloroform                        | 56.1                   | 2.8               | 97.2               |
| Carbon tetrachloride              | 42.6                   | 2.8               | 97.2               |
| Trichloroethylene                 | 73.4                   | 17                | 83                 |
| Tetrachloroethylene               | 88.5                   | 17.2              | 82.8               |
| 1,2-Dichloroethane                | 72                     | 8.3               | 91.7               |
| 1-Chloropropane                   | 44                     | 2.2               | 97.8               |
| 1,2-Dichloropropane               | 78                     | 12                | 88                 |
| Chlorobenzene                     | 90.2                   | 28.4              | 71.6               |
| Esters                            |                        |                   |                    |
| Ethyl formate                     | 52.6                   | 5                 | 95                 |
| Isopropyl formate                 | 65.0                   | 3                 | 97                 |
| Propyl formate                    | 71.6                   | 2.3               | 97.7               |
| Isobutyl formate                  | 80.4                   | 7.8               | 92.2               |
| Butyl formate                     | 83.8                   | 14.5              | 85.5               |
| Isopentyl formate                 | 90.2                   | 21                | 79                 |
| Pentyl formate                    | 91.6                   | 28.4              | 71.6               |
| Benzyl formate                    | 99.2                   | 80                | 20                 |
| Ethyl acetate                     | 70.38                  | 8.47              | 91.53              |
| Allyl acetate                     | 83                     | 14.7              | 85.3               |



**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                      | BP of azeotrope,<br>°C | Composition, wt % |                    |
|-----------------------------|------------------------|-------------------|--------------------|
|                             |                        | Water             | Other<br>component |
| Esters ( <i>continued</i> ) |                        |                   |                    |
| Isopropyl acetate           | 76.6                   | 10.6              | 89.4               |
| Propyl acetate              | 82.4                   | 14                | 86                 |
| Isobutyl acetate            | 87.4                   | 16.5              | 83.5               |
| Butyl acetate               | 90.2                   | 28.7              | 71.3               |
| Isopentyl acetate           | 93.8                   | 36.3              | 63.7               |
| Pentyl acetate              | 95.2                   | 41                | 59                 |
| Hexyl acetate               | 97.4                   | 61                | 39                 |
| Phenyl acetate              | 98.9                   | 75.1              | 24.9               |
| Benzyl acetate              | 99.6                   | 87.5              | 12.5               |
| Methyl propionate           | 71.4                   | 3.9               | 96.1               |
| Ethyl propionate            | 81.2                   | 10                | 90                 |
| Isopropyl propionate        | 85.2                   | 19.9              | 80.1               |
| Propyl propionate           | 88.9                   | 23                | 77                 |
| Isobutyl propionate         | 92.75                  | 52.2              | 47.8               |
| Isopentyl propionate        | 96.55                  | 48.5              | 51.5               |
| Methyl butyrate             | 82.7                   | 11.5              | 88.5               |
| Ethyl butyrate              | 87.9                   | 21.5              | 78.5               |
| Propyl butyrate             | 94.1                   | 36.4              | 63.6               |
| Isobutyl butyrate           | 96.3                   | 46                | 54                 |
| Butyl butyrate              | 97.2                   | 53                | 47                 |
| Isopentyl butyrate          | 98.05                  | 63.5              | 36.5               |
| Methyl isobutyrate          | 77.7                   | 6.8               | 93.2               |
| Ethyl isobutyrate           | 85.2                   | 15.2              | 84.8               |
| Propyl isobutyrate          | 92.2                   | 30.8              | 69.2               |
| Isobutyl isobutyrate        | 95.5                   | 39.4              | 60.6               |
| Isopentyl isobutyrate       | 97.4                   | 56.0              | 44.0               |
| Methyl isopentanoate        | 87.2                   | 19.2              | 80.8               |
| Ethyl isopentanoate         | 92.2                   | 30.2              | 69.8               |
| Propyl isopentanoate        | 96.2                   | 45.2              | 54.8               |
| Isobutyl isopentanoate      | 97.4                   | 55.8              | 44.2               |
| Isopentyl isopentanoate     | 98.8                   | 74.1              | 25.9               |
| Ethyl pentanoate            | 94.5                   | 40                | 60                 |
| Ethyl hexanoate             | 97.2                   | 54                | 46                 |
| Methyl benzoate             | 99.08                  | 79.2              | 20.8               |
| Ethyl benzoate              | 99.4                   | 84.0              | 16.0               |
| Propyl benzoate             | 99.7                   | 90.9              | 9.1                |
| Butyl benzoate              | 99.9                   | 94                | 6                  |
| Isopentyl benzoate          | 99.9                   | 95.6              | 4.4                |
| Ethyl phenylacetate         | 99.7                   | 91.3              | 8.7                |
| Methyl cinnamate            | 99.9                   | 95.5              | 4.5                |
| Methyl phthalate            | 99.95                  | 97.5              | 2.5                |
| Diethyl o-phthalate         | 99.98                  | 98.0              | 2.0                |
| Ethyl chloroacetate         | 95.2                   | 45.1              | 54.9               |
| Butyl chloroacetate         | 98.12                  | 75.5              | 24.5               |
| Methyl acrylate             | 71                     | 7.2               | 92.8               |
| Isobutyl carbonate          | 98.6                   | 74                | 26                 |
| Ethyl crotonate             | 93.5                   | 38                | 62                 |
| Methyl lactate              | 99                     | 80                | 20                 |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                      | BP of azeotrope,<br>°C | Composition, wt % |                 |
|-----------------------------|------------------------|-------------------|-----------------|
|                             |                        | Water             | Other component |
| Esters ( <i>continued</i> ) |                        |                   |                 |
| 1,2-Ethanediol diacetate    | 99.7                   | 84.6              | 15.4            |
| Ethyl nitrate               | 74.35                  | 22                | 78              |
| Propyl nitrate              | 84.8                   | 20                | 80              |
| Isobutyl nitrate            | 89.0                   | 25                | 75              |
| Methyl sulfate              | 98.6                   | 73                | 27              |
| Ethers                      |                        |                   |                 |
| Ethyl vinyl ether           | 34.6                   | 1.5               | 98.5            |
| Diethyl ether               | 34.2                   | 1.3               | 98.7            |
| Ethyl propyl ether          | 59.5                   | 4                 | 96              |
| Diisopropyl ether           | 62.2                   | 4.5               | 95.5            |
| Butyl ethyl ether           | 76.6                   | 11.9              | 88.1            |
| Diisobutyl ether            | 88.6                   | 23                | 77              |
| Dibutyl ether               | 92.9                   | 33                | 67              |
| Diisopentyl ether           | 97.4                   | 54                | 46              |
| 1,1-Diethoxyethane          | 82.6                   | 14.5              | 85.5            |
| Diphenyl ether              | 99.33                  | 96.75             | 3.25            |
| Methoxybenzene              | 95.5                   | 40.5              | 59.5            |
| Hydrocarbons                |                        |                   |                 |
| Pentane                     | 34.6                   | 1.4               | 98.6            |
| Hexane                      | 61.6                   | 5.6               | 94.4            |
| Heptane                     | 79.2                   | 12.9              | 87.1            |
| 2,2,4-Trimethylpentane      | 78.8                   | 11.1              | 88.9            |
| Nonane                      | 94.8                   | 82                | 18              |
| Undecane                    | 98.85                  | 96.0              | 4.0             |
| Dodecane                    | 99.45                  | 98                | 2               |
| Acrolein                    | 52.4                   | 2.6               | 97.4            |
| Cyclohexene                 | 70.8                   | 8.93              | 91.07           |
| Cyclohexane                 | 69.5                   | 8.4               | 91.6            |
| 1-Octene                    | 88.0                   | 28.7              | 71.3            |
| Benzene                     | 69.25                  | 8.83              | 91.17           |
| Toluene                     | 84.1                   | 13.5              | 86.5            |
| Ethylbenzene                | 92.0                   | 33.0              | 67.0            |
| <i>m</i> -Xylene            | 92                     | 35.8              | 64.2            |
| Isopropylbenzene            | 95                     | 43.8              | 56.2            |
| Naphthalene                 | 98.8                   | 84                | 16              |
| Ketones                     |                        |                   |                 |
| Acetone                     | zeotrope               |                   |                 |
| 2-Butanone                  | 73.5                   | 11                | 89              |
| 2-Pentanone                 | 83.3                   | 19.5              | 80.5            |
| Cyclopentanone              | 94.6                   | 42.4              | 57.6            |
| 4-Methyl-2-pentanone        | 87.9                   | 24.3              | 75.7            |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                                               | BP of azeotrope,<br>°C | Composition, wt % |                    |
|------------------------------------------------------|------------------------|-------------------|--------------------|
|                                                      |                        | Water             | Other<br>component |
| Ketones ( <i>continued</i> )                         |                        |                   |                    |
| 2-Heptanone                                          | 95                     | 48                | 52                 |
| 3-Heptanone                                          | 94.6                   | 42.2              | 57.8               |
| 4-Heptanone                                          | 94.3                   | 40.5              | 59.5               |
| 4-Hydroxy-4-methyl-2-pentanone                       | 98.8                   | 87.3              | 12.7               |
| 4-Methyl-3-penten-2-one                              | 91.8                   | 34.8              | 65.2               |
| Nitriles                                             |                        |                   |                    |
| Acetonitrile                                         | 76.5                   | 16.3              | 83.7               |
| Isobutyronitrile                                     | 82.5                   | 23                | 177                |
| Butyronitrile                                        | 88.7                   | 32.5              | 67.5               |
| Acrylonitrile                                        | 70.6                   | 14.3              | 85.7               |
| Miscellaneous                                        |                        |                   |                    |
| Hydrazine                                            | 120                    | 32.3              | 67.7               |
| Acetamide                                            | zeotrope               |                   |                    |
| Nitromethane                                         | 83.59                  | 23.6              | 76.4               |
| Nitroethane                                          | 87.22                  | 28.5              | 71.5               |
| 2,5-Dimethylfuran                                    | 77.0                   | 11.7              | 88.3               |
| Trioxane                                             | 91.4                   | 30                | 70                 |
| Carbon disulfide                                     | 42.6                   | 2.8               | 97.2               |
| <b>B. Binary azeotropes containing organic acids</b> |                        |                   |                    |
| System                                               | BP of azeotrope,<br>°C | Composition, wt % |                    |
|                                                      |                        | Acid              | Other<br>component |
| Formic acid                                          |                        |                   |                    |
| 2-Methylbutane                                       | 27.2                   | 4                 | 96                 |
| Pentane                                              | 34.2                   | 20                | 80                 |
| Hexane                                               | 60.6                   | 28                | 72                 |
| Methylcyclopentane                                   | 63.3                   | 29                | 71                 |
| Cyclohexane                                          | 70.7                   | 70                | 30                 |
| Methylcyclohexane                                    | 80.2                   | 46.5              | 53.5               |
| Heptane                                              | 78.2                   | 56.5              | 43.5               |
| Octane                                               | 90.5                   | 63                | 37                 |
| Benzene                                              | 71.05                  | 31                | 69                 |
| Toluene                                              | 85.8                   | 50                | 50                 |
| <i>o</i> -Xylene                                     | 95.5                   | 74                | 26                 |
| <i>m</i> -Xylene                                     | 92.8                   | 71.8              | 28.2               |
| Styrene                                              | 97.8                   | 73                | 27                 |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                           | BP of azeotrope,<br>°C | Composition, wt % |                 |
|----------------------------------|------------------------|-------------------|-----------------|
|                                  |                        | Acid              | Other component |
| Formic acid ( <i>continued</i> ) |                        |                   |                 |
| Iodomethane                      | 42.1                   | 6                 | 94              |
| Chloroform                       | 59.15                  | 15                | 85              |
| Carbon tetrachloride             | 66.65                  | 18.5              | 81.5            |
| Trichloroethylene                | 74.1                   | 25                | 75              |
| Tetrachloroethylene              | 88.2                   | 50                | 50              |
| Bromoethane                      | 38.2                   | 3                 | 97              |
| 1,2-Dibromoethane                | 94.7                   | 51.5              | 48.5            |
| 1,2-Dichloroethane               | 77.4                   | 14                | 86              |
| 1-Bromopropane                   | 64.7                   | 27                | 73              |
| 2-Bromopropane                   | 56.0                   | 14                | 86              |
| 1-Chloropropane                  | 45.6                   | 8                 | 92              |
| 2-Chloropropane                  | 34.7                   | 1.5               | 98.5            |
| 1-Chloro-2-methylpropane         | 63.0                   | 19                | 81              |
| Bromobenzene                     | 98.1                   | 68                | 32              |
| Chlorobenzene                    | 93.7                   | 59                | 41              |
| Fluorobenzene                    | 73.0                   | 27                | 73              |
| <i>o</i> -Chlorotoluene          | 100.2                  | 83                | 17              |
| Pyridine                         | 127.43                 | 61.4              | 38.6            |
| 2-Methylpyridine                 | 158.0                  | 25                | 75              |
| 2-Pentanone                      | 105.3                  | 32                | 68              |
| 3-Pentanone                      | 105.4                  | 33                | 67              |
| Nitromethane                     | 97.07                  | 45.5              | 54.5            |
| Diethyl sulfide                  | 82.2                   | 35                | 65              |
| Diisopropyl sulfide              | 93.5                   | 62                | 38              |
| Dipropyl sulfide                 | 98.0                   | 83                | 17              |
| Carbon disulfide                 | 42.55                  | 17                | 83              |
| Acetic acid                      |                        |                   |                 |
| Hexane                           | 68.3                   | 6.0               | 94.0            |
| Heptane                          | 91.7                   | 23                | 67              |
| Octane                           | 105.7                  | 53.7              | 46.3            |
| Nonane                           | 112.9                  | 69                | 31              |
| Decane                           | 116.75                 | 79.5              | 20.5            |
| Undecane                         | 117.9                  | 95                | 5               |
| Cyclohexane                      | 78.8                   | 9.6               | 90.4            |
| Methylcyclohexane                | 96.3                   | 31                | 69              |
| Benzene                          | 80.05                  | 2.0               | 98.0            |
| Toluene                          | 100.6                  | 28.1              | 71.9            |
| <i>o</i> -Xylene                 | 116.6                  | 78                | 22              |
| <i>m</i> -Xylene                 | 115.35                 | 72.5              | 27.5            |
| <i>p</i> -Xylene                 | 115.25                 | 72                | 28              |
| Ethylbenzene                     | 114.65                 | 66                | 34              |
| Styrene                          | 116.8                  | 85.7              | 14.3            |
| Isopropylbenzene                 | 116.0                  | 84                | 16              |
| Triethylamine                    | 163                    | 67                | 33              |
| Nitromethane                     | 101.2                  | 96                | 4               |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                           | BP of azeotrope,<br>°C | Composition, wt % |                    |
|----------------------------------|------------------------|-------------------|--------------------|
|                                  |                        | Acid              | Other<br>component |
| Acetic acid ( <i>continued</i> ) |                        |                   |                    |
| Nitroethane                      | 112.4                  | 30                | 70                 |
| Pyridine                         | 138.1                  | 51.1              | 48.9               |
| 2-Methylpyridine                 | 144.1                  | 40.4              | 59.6               |
| 3-Methylpyridine                 | 152.5                  | 30.4              | 69.6               |
| 4-Methylpyridine                 | 154.3                  | 30.3              | 69.7               |
| 2,6-Dimethylpyridine             | 148.1                  | 22.9              | 77.1               |
| Carbon tetrachloride             | 76                     | 98.46             | 1.54               |
| Trichloroethylene                | 86.5                   | 96.2              | 3.8                |
| Tetrachloroethylene              | 107.4                  | 61.5              | 38.5               |
| 1,2-Dibromoethane                | 114.4                  | 55                | 45                 |
| 2-Iodopropane                    | 88.3                   | 9                 | 91                 |
| 1-Bromobutane                    | 97.6                   | 18                | 82                 |
| 1-Bromo-2-methylpropane          | 90.2                   | 12                | 88                 |
| Chlorobenzene                    | 114.7                  | 58.5              | 41.5               |
| Trichloronitromethane            | 107.65                 | 80.5              | 19.5               |
| 1,4-Dioxane                      | 119.5                  | 77                | 23                 |
| Diisopropyl sulfide              | 111.5                  | 48                | 52                 |
| Propionic acid                   |                        |                   |                    |
| Heptane                          | 97.8                   | 2                 | 98                 |
| Octane                           | 120.9                  | 21.5              | 78.5               |
| Nonane                           | 134.3                  | 54.0              | 46.0               |
| Decane                           | 139.8                  | 80.5              | 19.5               |
| <i>o</i> -Xylene                 | 135.4                  | 43                | 57                 |
| <i>p</i> -Xylene                 | 132.5                  | 34                | 66                 |
| 1,3,5-Trimethylbenzene           | 139.3                  | 77                | 23                 |
| Isopropylbenzene                 | 139.0                  | 65                | 35                 |
| Propylbenzene                    | 139.5                  | 75                | 25                 |
| Camphene                         | 138.0                  | 65                | 35                 |
| $\alpha$ -Pinene                 | 136.4                  | 58.5              | 41.5               |
| Methoxybenzene                   | 140.8                  | 96                | 4                  |
| Pyridine                         | 148.6                  | 67.2              | 32.8               |
| 2-Methylpyridine                 | 154.5                  | 55.0              | 45.0               |
| 1,2-Dibromoethane                | 127.8                  | 17.5              | 82.5               |
| 1-Iodo-2-methylpropane           | 119.5                  | 9                 | 91                 |
| Chlorobenzene                    | 128.9                  | 18                | 82                 |
| Dipropyl sulfide                 | 136.5                  | 45                | 55                 |
| Butyric acid                     |                        |                   |                    |
| Undecane                         | 162.4                  | 84.4              | 15.5               |
| <i>o</i> -Xylene                 | 143.0                  | 10                | 90                 |
| <i>m</i> -Xylene                 | 138.5                  | 6                 | 94                 |
| <i>p</i> -Xylene                 | 137.8                  | 5.5               | 94.5               |
| Ethylbenzene                     | 135.8                  | 4                 | 96                 |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                            | BP of azeotrope,<br>°C | Composition, wt % |                    |
|-----------------------------------|------------------------|-------------------|--------------------|
|                                   |                        | Acid              | Other<br>component |
| Butyric acid ( <i>continued</i> ) |                        |                   |                    |
| Styrene                           | 143.5                  | 15                | 85                 |
| 1,2,4-Trimethylbenzene            | 159.5                  | 45                | 55                 |
| 1,3,5-Trimethylbenzene            | 158.0                  | 38                | 62                 |
| Isopropylbenzene                  | 149.5                  | 20                | 80                 |
| Propylbenzene                     | 154.5                  | 28                | 72                 |
| Butylbenzene                      | 162.5                  | 75                | 25                 |
| Naphthalene                       | zeotrope               |                   |                    |
| Indene                            | 163.7                  | 84                | 16                 |
| Camphene                          | 152.3                  | 2.8               | 97.2               |
| Methoxybenzene                    | 152.9                  | 12                | 88                 |
| Pyridine                          | 163.2                  | 92.0              | 8.0                |
| 2-Furaldehyde                     | 159.4                  | 42.5              | 57.5               |
| 1,2-Dibromoethane                 | 131.1                  | 3.5               | 96.5               |
| 1-Iodobutane                      | 129.8                  | 2.5               | 97.5               |
| Chlorobenzene                     | 131.75                 | 2.8               | 97.2               |
| 1,4-Dichlorobenzene               | 162.0                  | 57                | 43                 |
| <i>o</i> -Bromotoluene            | 163.0                  | 72                | 28                 |
| <i>m</i> -Bromotoluene            | 163.6                  | 79.5              | 20.5               |
| <i>p</i> -Bromotoluene            | 161.5                  | 75                | 25                 |
| $\alpha$ -Chlorotoluene           | 160.8                  | 65                | 35                 |
| Ethyl bromoacetate                | 157.4                  | 84                | 16                 |
| Propyl chloroacetate              | 160.5                  | 40                | 60                 |
| Isobutyric acid                   |                        |                   |                    |
| 2,7-Dimethyloctane                | 148.6                  | 48                | 52                 |
| <i>o</i> -Xylene                  | 141.0                  | 22                | 78                 |
| <i>m</i> -Xylene                  | 139.9                  | 15                | 85                 |
| <i>p</i> -Xylene                  | 136.4                  | 13                | 87                 |
| Styrene                           | 142.0                  | 27                | 73                 |
| 1,2,4-Trimethylbenzene            | 152.3                  | 63                | 37                 |
| Isopropylbenzene                  | 146.8                  | 35                | 65                 |
| Propylbenzene                     | 149.3                  | 49                | 51                 |
| Camphene                          | 148.1                  | 45                | 55                 |
| D-Limonene                        | 152.5                  | 78                | 22                 |
| Methoxybenzene                    | 149.0                  | 42                | 58                 |
| Ethyl bromoacetate                | 153.0                  | 40                | 60                 |
| Ethyl 2-oxopropionate             | 153.0                  | 60                | 40                 |
| 1,2-Dibromoethane                 | 130.5                  | 6.5               | 93.5               |
| 1-Iodobutane                      | 128.8                  | 7                 | 93                 |
| 1-Bromohexane                     | 148.0                  | 35                | 65                 |
| Bromobenzene                      | 148.6                  | 35                | 65                 |
| Chlorobenzene                     | 131.5                  | 8                 | 92                 |
| <i>o</i> -Bromotoluene            | 153.9                  | 85                | 15                 |
| $\alpha$ -Chlorotoluene           | 153.5                  | 80                | 20                 |
| Diisopentyl ether                 | 154.2                  | 93                | 7                  |
| Ethyl bromoacetate                | 153.0                  | 40                | 60                 |

TABLE 5.11 Binary Azeotropic (Constant-Boiling) Mixtures (Continued)

| C. Binary azeotropes containing alcohol |                     |                   |                 |
|-----------------------------------------|---------------------|-------------------|-----------------|
| System                                  | BP of azeotrope, °C | Composition, wt % |                 |
|                                         |                     | Alcohol           | Other component |
| Methanol                                |                     |                   |                 |
| Pentane                                 | 30.9                | 7                 | 93              |
| Cyclopentane                            | 38.8                | 14                | 86              |
| Cyclohexane                             | 53.9                | 36.4              | 63.6            |
| Methylcyclohexane                       | 59.2                | 54                | 46              |
| Heptane                                 | 59.1                | 51.5              | 48.5            |
| Octane                                  | 62.8                | 67.5              | 32.5            |
| Nonane                                  | 64.1                | 83.4              | 16.6            |
| Benzene                                 | 57.5                | 39.1              | 60.9            |
| Fluorobenzene                           | 59.7                | 32                | 68              |
| Toluene                                 | 63.5                | 72.5              | 27.5            |
| Bromomethane                            | 3.55                | 99.55             | 0.45            |
| Iodomethane                             | 37.8                | 95.5              | 4.5             |
| Bromodichloromethane                    | 63.8                | 60                | 40              |
| Chloroform                              | 53.4                | 87.4              | 12.6            |
| Carbon tetrachloride                    | 55.7                | 79.44             | 20.56           |
| Bromoethane                             | 34.9                | 5.3               | 94.7            |
| 1,2-Dichloroethane                      | 61.0                | 32                | 68              |
| Trichloroethylene                       | 59.3                | 38                | 62              |
| 1-Bromopropane                          | 54.5                | 21                | 79              |
| 2-Bromopropane                          | 48.6                | 15.0              | 85.0            |
| 1-Chloropropane                         | 40.5                | 9.5               | 90.5            |
| 2-Chloropropane                         | 33.4                | 6                 | 94              |
| 2-Iodopropane                           | 61.0                | 38                | 62              |
| 1-Chlorobutane                          | 57.0                | 27                | 73              |
| Isobutyl formate                        | 64.6                | 95                | 5               |
| Methyl acetate                          | 53.5                | 19                | 81              |
| Methyl acrylate                         | 62.5                | 54                | 46              |
| Methyl nitrate                          | 52.5                | 73                | 27              |
| Acetone                                 | 55.5                | 12.1              | 87.9            |
| 1,4-Dioxane                             | zeotrope            |                   |                 |
| Dipropyl ether                          | 63.8                | 72                | 28              |
| Methyl <i>tert</i> -butyl ether         | 51.3                | 14.3              | 85.7            |
| Diethyl sulfide                         | 61.2                | 62                | 38              |
| Carbon disulfide                        | 39.8                | 71                | 29              |
| Thiophene                               | 59.7                | 16.4              | 83.6            |
| Nitromethane                            | 64.4                | 9.1               | 90.9            |
| Ethanol                                 |                     |                   |                 |
| Pentane                                 | 34.3                | 5                 | 95              |
| Cyclopentane                            | 44.7                | 7.5               | 92.5            |
| Hexane                                  | 58.7                | 21                | 79              |
| Cyclohexane                             | 64.8                | 29.2              | 70.8            |
| Heptane                                 | 70.9                | 49                | 51              |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                       | BP of azeotrope,<br>°C | Composition, wt % |                 |
|------------------------------|------------------------|-------------------|-----------------|
|                              |                        | Alcohol           | Other component |
| Ethanol ( <i>continued</i> ) |                        |                   |                 |
| Octane                       | 77.0                   | 78                | 22              |
| Benzene                      | 67.9                   | 31.7              | 68.3            |
| Fluorobenzene                | 70.0                   | 75                | 25              |
| Toluene                      | 76.7                   | 68                | 32              |
| Bromodichloromethane         | 75.5                   | 72                | 28              |
| Iodomethane                  | 41.2                   | 96.8              | 3.2             |
| Chloroform                   | 59.3                   | 93                | 7               |
| Trichloronitromethane        | 77.5                   | 34                | 66              |
| Carbon tetrachloride         | 65.0                   | 84.2              | 15.8            |
| 1,2-Dichloroethane           | 70.5                   | 37                | 63              |
| 3-Chloro-1-propene           | 44                     | 5                 | 95              |
| 1-Bromopropane               | 62.8                   | 20.5              | 79.5            |
| 2-Bromopropane               | 55.6                   | 10.5              | 89.5            |
| 1-Chloropropane              | 45.0                   | 6                 | 94              |
| 2-Chloropropane              | 35.6                   | 2.8               | 97.2            |
| 1-Iodopropane                | 75.4                   | 44                | 56              |
| 2-Iodopropane                | 71.5                   | 27                | 73              |
| 1-Bromobutane                | 75.0                   | 43                | 57              |
| 1-Chlorobutane               | 65.7                   | 20.3              | 79.7            |
| 2-Butanone                   | 74.8                   | 40                | 60              |
| 1,1-Diethoxyethane           | 78.0                   | 76                | 24              |
| Dipropyl ether               | 74.5                   | 44                | 56              |
| Acetronitrile                | 72.5                   | 44                | 56              |
| Acrylonitrile                | 70.8                   | 41                | 59              |
| Nitromethane                 | 76.1                   | 29                | 71              |
| Carbon disulfide             | 42.6                   | 91                | 9               |
| Diethyl sulfide              | 72.6                   | 56                | 44              |
| 1-Propanol                   |                        |                   |                 |
| Hexane                       | 65.7                   | 4                 | 96              |
| Cyclohexane                  | 74.7                   | 18.5              | 81.5            |
| Methylcyclohexane            | 87.0                   | 34.7              | 65.3            |
| Heptane                      | 84.6                   | 34.7              | 65.3            |
| Octane                       | 93.9                   | 70                | 30              |
| Benzene                      | 77.1                   | 16.9              | 83.1            |
| Toluene                      | 92.5                   | 51.2              | 48.8            |
| <i>o</i> -Xylene             | zeotrope               |                   |                 |
| <i>m</i> -Xylene             | 97.1                   | 94                | 6               |
| <i>p</i> -Xylene             | 96.9                   | 92.2              | 7.8             |
| Styrene                      | 97.0                   | 8                 | 92              |
| Propyl formate               | 80.7                   | 3                 | 97              |
| Butyl formate                | 95.5                   | 64                | 36              |
| Propyl acetate               | 94.7                   | 51                | 49              |
| Ethyl propionate             | 93.4                   | 48                | 52              |
| Methyl butyrate              | 94.4                   | 49                | 51              |
| Dipropyl ether               | 85.7                   | 30                | 70              |



**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                          | BP of azeotrope,<br>°C | Composition, wt % |                    |
|---------------------------------|------------------------|-------------------|--------------------|
|                                 |                        | Alcohol           | Other<br>component |
| 1-Propanol ( <i>continued</i> ) |                        |                   |                    |
| 1,1-Diethoxyethane              | 92.4                   | 37                | 63                 |
| 1,4-Dioxane                     | 95.3                   | 55                | 45                 |
| Chloroform                      | zeotrope               |                   |                    |
| Carbon tetrachloride            | 73.4                   | 92.1              | 7.9                |
| Trichloronitromethane           | 94.1                   | 58.5              | 41.5               |
| Iodoethane                      | 70                     | 93                | 7                  |
| 1,2-Dichloroethane              | 80.7                   | 19                | 81                 |
| Tetrachloroethylene             | 94.0                   | 52                | 48                 |
| 1-Bromopropane                  | 69.7                   | 9                 | 91                 |
| 1-Chlorobutane                  | 74.8                   | 18                | 82                 |
| Chlorobenzene                   | 96.5                   | 80                | 20                 |
| Fluorobenzene                   | 80.2                   | 18                | 82                 |
| Nitromethane                    | 89.1                   | 48.4              | 51.6               |
| 1-Nitropropane                  | 97.0                   | 8.8               | 91.2               |
| Carbon disulfide                | 45.7                   | 94.5              | 5.5                |
| 2-Propanol                      |                        |                   |                    |
| Pentane                         | 35.5                   | 6                 | 94                 |
| Hexane                          | 62.7                   | 23                | 77                 |
| Cyclohexane                     | 69.4                   | 32                | 68                 |
| Heptane                         | 76.4                   | 50.5              | 49.5               |
| Octane                          | 81.6                   | 84                | 16                 |
| Benzene                         | 71.7                   | 33.7              | 66.3               |
| Fluorobenzene                   | 74.5                   | 30                | 70                 |
| Toluene                         | 80.6                   | 69                | 31                 |
| Chloroform                      | 60.8                   | 4.2               | 95.8               |
| Trichloronitromethane           | 81.9                   | 35                | 65                 |
| Carbon tetrachloride            | 69.0                   | 18                | 82                 |
| 1,2-Dichloroethane              | 74.7                   | 43.5              | 56.5               |
| Iodoethane                      | 67.1                   | 15                | 85                 |
| 3-Bromo-1-propene               | 66.5                   | 20                | 80                 |
| 1-Chloropropane                 | 46.4                   | 2.8               | 97.2               |
| 1-Bromopropane                  | 66.8                   | 20.5              | 79.5               |
| 2-Bromopropane                  | 57.8                   | 12                | 88                 |
| 1-Iodopropane                   | 79.8                   | 42                | 58                 |
| 2-Iodopropane                   | 76.0                   | 32                | 68                 |
| 1-Chlorobutane                  | 70.8                   | 23                | 77                 |
| Ethyl acetate                   | 75.3                   | 25                | 75                 |
| Isopropyl acetate               | 81.3                   | 60                | 40                 |
| Methyl propionate               | 76.4                   | 37                | 63                 |
| Acrylonitrile                   | 71.7                   | 56                | 44                 |
| Butylamine                      | 74.7                   | 60                | 40                 |
| 2-Butanone                      | 77.5                   | 32                | 68                 |
| 1,1-Diethoxyethane              | 81.3                   | 63                | 37                 |
| Ethyl propyl ether              | 62.0                   | 10                | 90                 |
| Diisopropyl ether               | 66.2                   | 14.1              | 85.9               |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                  | BP of azeotrope,<br>°C | Composition, wt % |                    |
|-------------------------|------------------------|-------------------|--------------------|
|                         |                        | Alcohol           | Other<br>component |
| 1-Butanol               |                        |                   |                    |
| Cyclohexane             | 79.8                   | 9.5               | 90.5               |
| Cyclohexene             | 82.0                   | 5                 | 95                 |
| Hexane                  | 68.2                   | 3.2               | 96.8               |
| Methylcyclohexane       | 95.3                   | 20                | 80                 |
| Heptane                 | 93.9                   | 18                | 82                 |
| Octane                  | 108.5                  | 45.2              | 54.8               |
| Nonane                  | 115.9                  | 71.5              | 28.5               |
| Toluene                 | 105.5                  | 27.8              | 72.2               |
| <i>o</i> -Xylene        | 116.8                  | 75                | 25                 |
| <i>m</i> -Xylene        | 116.5                  | 71.5              | 28.5               |
| <i>p</i> -Xylene        | 115.7                  | 68                | 32                 |
| Ethylbenzene            | 115.9                  | 65.1              | 34.9               |
| Butyl formate           | 105.8                  | 23.6              | 76.4               |
| Isopentyl formate       | 115.9                  | 69                | 31                 |
| Butyl acetate           | 117.2                  | 47                | 53                 |
| Isobutyl acetate        | 114.5                  | 50                | 50                 |
| Ethyl butyrate          | 115.7                  | 64                | 36                 |
| Ethyl isobutyrate       | 109.2                  | 17                | 83                 |
| Methyl isopentanoate    | 113.5                  | 40                | 60                 |
| Ethyl borate            | 113.0                  | 52                | 48                 |
| Ethyl carbonate         | 116.5                  | 63                | 37                 |
| Isobutyl nitrate        | 112.8                  | 45                | 55                 |
| Dibutyl ether           | 117.8                  | 82.5              | 17.5               |
| Diisobutyl ether        | 113.5                  | 48                | 52                 |
| 1,1-Diethoxyethane      | 101.0                  | 13                | 87                 |
| Carbon tetrachloride    | 76.6                   | 97.6              | 2.4                |
| Tetrachloroethylene     | 110.0                  | 68                | 32                 |
| 2-Bromo-2-methylpropane | 90.2                   | 7                 | 93                 |
| 2-Iodo-2-methylpropane  | 110.5                  | 30                | 70                 |
| Chlorobenzene           | 115.3                  | 56                | 44                 |
| Paraldehyde             | 115.8                  | 52                | 48                 |
| Hexaldehyde             | 116.8                  | 77.1              | 22.9               |
| Ethylenediamine         | 124.7                  | 35.7              | 64.3               |
| Pyridine                | 118.6                  | 69                | 31                 |
| 1-Nitropropane          | 115.3                  | 32.2              | 67.8               |
| Butyronitrile           | 113.0                  | 50                | 50                 |
| Diisopropyl sulfide     | 112.0                  | 45                | 55                 |
| 2-Methyl-2-propanol     |                        |                   |                    |
| Cyclohexene             | 80.5                   | 14.2              | 85.8               |
| Cyclohexane             | 78.3                   | 14                | 86                 |
| Methylcyclopentane      | 71.0                   | 5                 | 95                 |
| Hexane                  | 68.3                   | 2.5               | 97.5               |
| Methylcyclohexane       | 92.6                   | 32                | 68                 |
| Heptane                 | 90.8                   | 27                | 73                 |
| 2,5-Dimethylhexane      | 98.7                   | 42                | 58                 |
| 1,3-Dimethylcyclohexane | 102.2                  | 56                | 44                 |
| 2,2,4-Trimethylpentane  | 92.0                   | 27                | 73                 |
| Benzene                 | 79.3                   | 7.4               | 92.6               |
| Chlorobenzene           | 107.1                  | 63                | 37                 |
| Fluorobenzene           | 84.0                   | 9                 | 91                 |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                                   | BP of azeotrope,<br>°C | Composition, wt % |                    |
|------------------------------------------|------------------------|-------------------|--------------------|
|                                          |                        | Alcohol           | Other<br>component |
| 2-Methyl-2-propanol ( <i>continued</i> ) |                        |                   |                    |
| Toluene                                  | 101.2                  | 45                | 55                 |
| Ethylbenzene                             | 107.2                  | 80                | 20                 |
| <i>p</i> -Xylene                         | 107.1                  | 88.6              | 11.4               |
| Butyl formate                            | 103.0                  | 40                | 60                 |
| Isobutyl formate                         | 97.4                   | 12                | 88                 |
| Propyl acetate                           | 101.0                  | 17                | 83                 |
| Isobutyl acetate                         | 107.6                  | 92                | 8                  |
| Methyl butyrate                          | 101.3                  | 25                | 75                 |
| Ethyl isobutyrate                        | 105.5                  | 52                | 48                 |
| Methyl chloroacetate                     | 107.6                  | 12                | 88                 |
| Dipropyl ether                           | 89.5                   | 10                | 90                 |
| Isobutyl vinyl ether                     | 82.7                   | 6.2               | 93.8               |
| 1,1-Diethoxyethane                       | 98.2                   | 20                | 80                 |
| 2-Pentanone                              | 101.8                  | 19                | 81                 |
| 3-Pentanone                              | 101.7                  | 20                | 80                 |
| 1,2-Dichloroethane                       | 83.5                   | 6.5               | 93.5               |
| 1-Bromobutane                            | 95.0                   | 21                | 79                 |
| 1-Chlorobutane                           | 77.7                   | 4                 | 96                 |
| 2-Bromo-2-methylpropane                  | 88.8                   | 12                | 88                 |
| 2-Iodo-2-methylpropane                   | 104.0                  | 36                | 64                 |
| 1-Nitropropane                           | 105.3                  | 15.2              | 84.8               |
| Isobutyl nitrate                         | 105.6                  | 36                | 64                 |
| Diisopropyl sulfide                      | 105.8                  | 73                | 27                 |
| 3-Methyl-1-butanol                       |                        |                   |                    |
| Heptane                                  | 97.7                   | 7                 | 93                 |
| Octane                                   | 117.0                  | 30                | 70                 |
| Toluene                                  | 109.7                  | 10                | 90                 |
| Ethylbenzene                             | 125.7                  | 49                | 51                 |
| Isopropylbenzene                         | 131.6                  | 94                | 6                  |
| Camphene                                 | 130.9                  | 24                | 76                 |
| Bromobenzene                             | 131.7                  | 85                | 15                 |
| <i>o</i> -Fluorotoluene                  | 112.1                  | 14.0              | 86.0               |
| Butyl acetate                            | 125.9                  | 16.5              | 83.5               |
| Paraldehyde                              | 123.5                  | 22.0              | 78.0               |
| Dibutyl ether                            | 129.8                  | 65                | 35                 |
| Cyclohexanol                             |                        |                   |                    |
| <i>o</i> -Xylene                         | 143.0                  | 14                | 86                 |
| <i>m</i> -Xylene                         | 138.9                  | 5                 | 95                 |
| Propylbenzene                            | 153.8                  | 40                | 60                 |
| Indene                                   | 160.0                  | 75                | 25                 |
| Camphene                                 | 151.9                  | 41                | 59                 |
| Cineole                                  | 160.6                  | 92                | 8                  |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                  | BP of azeotrope,<br>°C | Composition, wt % |                 |
|-------------------------|------------------------|-------------------|-----------------|
|                         |                        | Alcohol           | Other component |
| Allyl alcohol           |                        |                   |                 |
| Methylcyclohexane       | 85.0                   | 42                | 58              |
| Hexane                  | 65.5                   | 4.5               | 95.5            |
| Cyclohexane             | 74.0                   | 58                | 42              |
| 2,5-Dimethylhexane      | 89.3                   | 50                | 50              |
| Octane                  | 93.4                   | 68                | 32              |
| Benzene                 | 76.75                  | 17.36             | 82.64           |
| Toluene                 | 92.4                   | 50                | 50              |
| Propyl acetate          | 94.2                   | 53                | 47              |
| Methyl butyrate         | 93.8                   | 55                | 45              |
| 1,2-Dichloroethane      | 79.9                   | 18                | 82              |
| 3-Iodo-1-propene        | 89.4                   | 28                | 72              |
| Chlorobenzene           | 96.2                   | 85                | 15              |
| Diethyl sulfide         | 85.1                   | 45                | 55              |
| Phenol                  |                        |                   |                 |
| 2,7-Dimethyloctane      | 159.5                  | 6                 | 94              |
| Decane                  | 168.0                  | 35                | 65              |
| Tridecane               | 180.6                  | 83.1              | 16.9            |
| Butylbenzene            | 175.0                  | 46                | 54              |
| 1,2,4-Trimethylbenzene  | 166.0                  | 25                | 75              |
| 1,3,5-Trimethylbenzene  | 163.5                  | 21                | 79              |
| Indene                  | 177.8                  | 47                | 53              |
| Camphene                | 156.1                  | 22                | 78              |
| Benzaldehyde            | 175.6                  | 51.0              | 49.0            |
| 1-Octanol               | 195.4                  | 13                | 87              |
| 2-Octanol               | 184.5                  | 50                | 50              |
| Dipentyl ether          | 180.2                  | 78                | 22              |
| Diisopentyl ether       | 172.2                  | 15                | 85              |
| 2-Methylpyridine        | 185.5                  | 75.4              | 24.6            |
| 3-Methylpyridine        | 188.9                  | 71.2              | 29.8            |
| 4-Methylpyridine        | 190.0                  | 67.5              | 32.5            |
| 2,4-Dimethylpyridine    | 193.4                  | 57.0              | 43.0            |
| 2,6-Dimethylpyridine    | 185.5                  | 72.5              | 27.5            |
| 2,4,6-Trimethylpyridine | 195.2                  | 52.3              | 47.7            |
| Aniline                 | 185.8                  | 41.9              | 58.1            |
| Ethylene diacetate      | 195.5                  | 39.2              | 60.8            |
| Iodobenzene             | 177.7                  | 53                | 47              |
| Benzyl alcohol          |                        |                   |                 |
| Naphthalene             | 204.1                  | 60                | 40              |
| D-Limonene              | 176.4                  | 11                | 89              |
| 1,3,5-Triethylbenzene   | 203.2                  | 57                | 43              |
| <i>o</i> -Cresol        | zeotrope               |                   |                 |
| <i>m</i> -Cresol        | 207.1                  | 61                | 39              |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                              | BP of azeotrope,<br>°C | Composition, wt % |                    |
|-------------------------------------|------------------------|-------------------|--------------------|
|                                     |                        | Alcohol           | Other<br>component |
| Benzyl alcohol ( <i>continued</i> ) |                        |                   |                    |
| <i>p</i> -Cresol                    | 206.8                  | 62                | 38                 |
| <i>N</i> -Methylaniline             | 195.8                  | 30                | 70                 |
| <i>N,N</i> -Dimethylaniline         | 193.9                  | 6.5               | 93.5               |
| <i>N</i> -Ethylaniline              | 202.8                  | 50                | 50                 |
| <i>N,N</i> -Diethylaniline          | 204.2                  | 72                | 28                 |
| Iodobenzene                         | 187.8                  | 12                | 88                 |
| Nitrobenzene                        | 204.0                  | 58                | 42                 |
| <i>o</i> -Bromotoluene              | 181.3                  | 7                 | 93                 |
| Borneol                             | 205.1                  | 85.8              | 14.2               |
| 2-Ethoxyethanol                     |                        |                   |                    |
| Methylcyclohexane                   | 98.6                   | 15                | 85                 |
| Heptane                             | 96.5                   | 14                | 86                 |
| Octane                              | 116.0                  | 38                | 62                 |
| Toluene                             | 110.2                  | 10.8              | 89.2               |
| Ethylbenzene                        | 127.8                  | 48                | 52                 |
| <i>p</i> -Xylene                    | 128.6                  | 50                | 50                 |
| Styrene                             | 130.0                  | 55                | 45                 |
| Propylbenzene                       | 134.6                  | 80                | 20                 |
| Isopropylbenzene                    | 133.2                  | 67                | 33                 |
| Camphene                            | 131.0                  | 65                | 35                 |
| Propyl butyrate                     | 133.5                  | 72                | 28                 |
| 2-Butoxyethanol                     |                        |                   |                    |
| Dipentene                           | 164.0                  | 53                | 47                 |
| 1,3,5-Trimethylbenzene              | 162.0                  | 32                | 68                 |
| Butylbenzene                        | 169.6                  | 73.4              | 26.6               |
| Camphene                            | 154.5                  | 30                | 70                 |
| <i>o</i> -Cresol                    | 191.6                  | 15                | 85                 |
| Phenetole                           | 167.1                  | 52                | 48                 |
| Cineole                             | 168.9                  | 58.5              | 41.5               |
| Benzaldehyde                        | 171.0                  | 91                | 9                  |
| Diisobutyl sulfide                  | 163.8                  | 42                | 58                 |
| 1,2-Ethanediol                      |                        |                   |                    |
| Heptane                             | 97.9                   | 3                 | 97                 |
| Decane                              | 161.0                  | 23                | 77                 |
| Tridecane                           | 188.0                  | 55                | 45                 |
| Toluene                             | 110.1                  | 2.3               | 97.7               |
| Styrene                             | 139.5                  | 16.5              | 83.5               |
| Stilbene                            | 196.8                  | 87                | 13                 |
| <i>m</i> -Xylene                    | 135.1                  | 6.55              | 93.45              |
| <i>p</i> -Xylene                    | 134.5                  | 6.4               | 93.6               |
| 1,3,5-Trimethylbenzene              | 156                    | 13                | 87                 |
| Propylbenzene                       | 152                    | 19                | 81                 |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                              | BP of azeotrope,<br>°C | Composition, wt % |                 |
|-------------------------------------|------------------------|-------------------|-----------------|
|                                     |                        | Alcohol           | Other component |
| 1,2-Ethanediol ( <i>continued</i> ) |                        |                   |                 |
| Isopropylbenzene                    | 147.0                  | 18                | 82              |
| Naphthalene                         | 183.9                  | 51                | 49              |
| 1-Methylnaphthalene                 | 190.3                  | 60.0              | 40.0            |
| 2-Methylnaphthalene                 | 189.1                  | 57.2              | 42.8            |
| Anthracene                          | 197                    | 98.3              | 1.7             |
| Indene                              | 168.4                  | 26                | 74              |
| Acenaphthene                        | 194.65                 | 74.2              | 25.8            |
| Fluorene                            | 196.0                  | 82                | 18              |
| Camphene                            | 152.5                  | 20                | 80              |
| Camphor                             | 186.2                  | 40                | 60              |
| Biphenyl                            | 192.3                  | 66.5              | 33.5            |
| Diphenylmethane                     | 193.3                  | 68.5              | 31.5            |
| Benzyl alcohol                      | 193.1                  | 56                | 44              |
| 2-Phenylethanol                     | 194.4                  | 69                | 31              |
| <i>o</i> -Cresol                    | 189.6                  | 27                | 73              |
| <i>m</i> -Cresol                    | 195.2                  | 60                | 40              |
| 3,4-Dimethylphenol                  | 197.2                  | 89                | 11              |
| Menthol                             | 188.6                  | 51.5              | 48.5            |
| Ethyl benzoate                      | 186.1                  | 46.5              | 53.5            |
| <i>o</i> -Bromotoluene              | 166.8                  | 25                | 75              |
| Dibutyl ether                       | 139.5                  | 6.4               | 93.6            |
| Methoxybenzene                      | 150.5                  | 10.5              | 89.5            |
| Diphenyl ether                      | 193.1                  | 60                | 40              |
| Benzyl phenyl ether                 | 195.5                  | 87                | 13              |
| Acetophenone                        | 185.7                  | 52                | 48              |
| 2,4-Dimethylaniline                 | 188.6                  | 47                | 53              |
| <i>N,N</i> -Dimethylaniline         | 175.9                  | 33.5              | 66.5            |
| <i>m</i> -Toluidine                 | 188.6                  | 42                | 58              |
| 2,4,6-Trimethylpyridine             | 170.5                  | 9.7               | 90.3            |
| Quinoline                           | 196.4                  | 79.5              | 20.5            |
| Tetrachloroethylene                 | 119.1                  | 94                | 6               |
| 1,2-Dibromoethane                   | 129.8                  | 4                 | 96              |
| Chlorobenzene                       | 130.1                  | 94.4              | 5.6             |
| $\alpha$ -Chlorotoluene             | 167.0                  | 30                | 70              |
| Nitrobenzene                        | 185.9                  | 59                | 41              |
| <i>o</i> -Nitrotoluene              | 188.5                  | 48.5              | 51.5            |
| 1,2-Ethanediol monoacetate          |                        |                   |                 |
| Indene                              | 180.0                  | 20                | 80              |
| 1-Octanol                           | 189.5                  | 71                | 29              |
| Phenol                              | 197.5                  | 65                | 35              |
| <i>o</i> -Cresol                    | 199.5                  | 51                | 49              |
| <i>m</i> -Cresol                    | 206.5                  | 31                | 69              |
| <i>p</i> -Cresol                    | 206.0                  | 33                | 67              |
| Dipentyl ether                      | 180.8                  | 42                | 58              |
| Diisopentyl ether                   | 170.2                  | 28                | 72              |
| <i>m</i> -Bromotoluene              | 182.0                  | 32                | 68              |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| D. Binary azeotropes containing ketones |                        |                   |                 |
|-----------------------------------------|------------------------|-------------------|-----------------|
| System                                  | BP of azeotrope,<br>°C | Composition, wt % |                 |
|                                         |                        | Ketone            | Other component |
| Acetone                                 |                        |                   |                 |
| Cyclopentane                            | 41.0                   | 36                | 64              |
| Pentane                                 | 32.5                   | 20                | 80              |
| Cyclohexane                             | 53.0                   | 67.5              | 32.5            |
| Hexane                                  | 49.8                   | 59                | 41              |
| Heptane                                 | 55.9                   | 89.5              | 10.5            |
| Diethylamine                            | 51.4                   | 38.2              | 61.8            |
| Methyl acetate                          | 55.8                   | 48.3              | 51.7            |
| Diisopropyl ether                       | 54.2                   | 61                | 39              |
| Chloroform                              | 64.4                   | 78.1              | 21.9            |
| Carbon tetrachloride                    | 56.1                   | 11.5              | 88.5            |
| Carbon disulfide                        | 39.3                   | 67                | 33              |
| Ethylene sulfide                        | 51.5                   | 57                | 43              |
| 2-Butanone                              |                        |                   |                 |
| Cyclohexane                             | 71.8                   | 40                | 60              |
| Hexane                                  | 64.2                   | 28.6              | 71.4            |
| Heptane                                 | 77.0                   | 70                | 30              |
| 2,5-Dimethylhexane                      | 79.0                   | 95                | 5               |
| Benzene                                 | 78.33                  | 44                | 56              |
| 2-Methyl-2-propanol                     | 78.7                   | 69                | 31              |
| Butylamine                              | 74.0                   | 35                | 65              |
| Ethyl acetate                           | 77.1                   | 11.8              | 88.2            |
| Methyl propionate                       | 79.0                   | 60                | 40              |
| Butyl nitrite                           | 76.7                   | 30                | 70              |
| 1-Chlorobutane                          | 77.0                   | 38                | 62              |
| Fluorobenzene                           | 79.3                   | 75                | 25              |
| E. Miscellaneous binary azeotropes      |                        |                   |                 |
| System                                  | BP of azeotrope,<br>°C | Composition, wt % |                 |
|                                         |                        | Solvent           | Other component |
| Solvent: acetamide                      |                        |                   |                 |
| Dipentene                               | 169.2                  | 18                | 82              |
| Biphenyl                                | 213.0                  | 50.5              | 49.5            |
| Diphenylmethane                         | 215.2                  | 56.5              | 43.5            |
| 1,2-Diphenylethane                      | 218.2                  | 68                | 32              |
| o-Xylene                                | 142.6                  | 11                | 89              |

**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                                  | BP of azeotrope,<br>°C | Composition, wt % |                 |
|-----------------------------------------|------------------------|-------------------|-----------------|
|                                         |                        | Solvent           | Other component |
| Solvent: acetamide ( <i>continued</i> ) |                        |                   |                 |
| <i>m</i> -Xylene                        | 138.4                  | 10                | 90              |
| <i>p</i> -Xylene                        | 137.8                  | 8                 | 92              |
| Styrene                                 | 144                    | 12                | 88              |
| 4-Isopropyl-1-methylbenzene             | 170.5                  | 19                | 81              |
| Naphthalene                             | 199.6                  | 27                | 73              |
| 1-Methylnaphthalene                     | 209.8                  | 43.8              | 56.2            |
| 2-Methylnaphthalene                     | 208.3                  | 40                | 60              |
| Indene                                  | 177.2                  | 17.5              | 82.5            |
| Acenaphthene                            | 217.1                  | 64.2              | 35.8            |
| Camphene                                | 155.5                  | 12                | 88              |
| Camphor                                 | 199.8                  | 23                | 77              |
| Benzaldehyde                            | 178.6                  | 6.5               | 93.5            |
| 3,4-Dimethylphenol                      | 221.1                  | 96                | 4               |
| 2-Methoxy-4-(2-propenyl)phenol          | 220.8                  | 88                | 12              |
| <i>N</i> -Methylaniline                 | 193.8                  | 14                | 86              |
| <i>N</i> -Ethylaniline                  | 199.0                  | 18                | 82              |
| <i>N,N</i> -Diethylaniline              | 198.1                  | 24                | 76              |
| Diphenyl ether                          | 214.6                  | 52                | 48              |
| Safrole                                 | 208.8                  | 32                | 68              |
| Tetrachloroethylene                     | 120.5                  | 97.4              | 2.6             |
| Solvent: aniline                        |                        |                   |                 |
| Nonane                                  | 149.2                  | 13.5              | 86.5            |
| Decane                                  | 167.3                  | 36                | 64              |
| Undecane                                | 175.3                  | 57.5              | 42.5            |
| Dodecane                                | 180.4                  | 71.5              | 28.5            |
| Tridecane                               | 182.9                  | 86.2              | 13.8            |
| Tetradecane                             | 183.9                  | 95.2              | 4.8             |
| Butylbenzene                            | 177.8                  | 46                | 54              |
| 1,2,4-Trimethylbenzene                  | 168.6                  | 13.5              | 86.5            |
| 1,3,5-Trimethylbenzene                  | 164.3                  | 12.0              | 88.0            |
| Indene                                  | 179.8                  | 41.5              | 58.5            |
| 1-Octanol                               | 183.9                  | 83                | 17              |
| <i>o</i> -Cresol                        | 191.3                  | 8                 | 92              |
| Dipentyl ether                          | 177.5                  | 55                | 45              |
| Diisopentyl ether                       | 169.3                  | 28                | 72              |
| Hexachloroethane                        | 176.8                  | 66                | 34              |
| Solvent: pyridine                       |                        |                   |                 |
| Heptane                                 | 95.6                   | 25.3              | 74.7            |
| Octane                                  | 109.5                  | 56.1              | 43.9            |
| Nonane                                  | 115.1                  | 89.9              | 10.1            |
| Toluene                                 | 110.1                  | 22.2              | 77.8            |
| Phenol                                  | 183.1                  | 13.1              | 86.9            |
| Piperidine                              | 106.1                  | 8                 | 92              |



**TABLE 5.11** Binary Azeotropic (Constant-Boiling) Mixtures (*Continued*)

| System                                | BP of azeotrope,<br>°C | Composition, wt % |                    |
|---------------------------------------|------------------------|-------------------|--------------------|
|                                       |                        | Solvent           | Other<br>component |
| Solvent: thiophene                    |                        |                   |                    |
| Methylcyclopentane                    | 71.5                   | 14                | 86                 |
| Cyclohexane                           | 77.9                   | 41.2              | 58.8               |
| Hexane                                | 68.5                   | 11.2              | 88.8               |
| Heptane                               | 83.1                   | 83.2              | 16.8               |
| 2,3-Dimethylpentane                   | 80.9                   | 64                | 36                 |
| 2,4-Dimethylpentane                   | 76.6                   | 42.7              | 57.3               |
| Solvent: benzene                      |                        |                   |                    |
| Methylcyclopentane                    | 71.7                   | 16                | 84                 |
| Cyclohexene                           | 78.9                   | 64.7              | 35.3               |
| Cyclohexane                           | 77.6                   | 51.9              | 48.1               |
| Hexane                                | 68.5                   | 4.7               | 95.3               |
| Heptane                               | 80.1                   | 99.3              | 0.7                |
| 2,2-Dimethylpentane                   | 75.9                   | 46.3              | 53.7               |
| 2,3-Dimethylpentane                   | 79.4                   | 78.8              | 21.2               |
| 2,4-Dimethylpentane                   | 75.2                   | 48.3              | 51.7               |
| 2,2,4-Trimethylpentane                | 80.1                   | 97.7              | 2.3                |
| Solvent: bis(2-hydroxyethyl) ether    |                        |                   |                    |
| Biphenyl                              | 232.7                  | 48                | 52                 |
| Diphenylmethane                       | 236.0                  | 52                | 48                 |
| 1,3,5-Trimethylbenzene                | 210.0                  | 22                | 78                 |
| Naphthalene                           | 212.6                  | 22                | 78                 |
| 1-Methylnaphthalene                   | 277.0                  | 45                | 55                 |
| 2-Methylnaphthalene                   | 225.5                  | 39                | 61                 |
| Acenaphthene                          | 239.6                  | 62                | 38                 |
| Fluorene                              | 243.0                  | 80                | 20                 |
| Benzyl acetate                        | 214.9                  | 7                 | 93                 |
| Bornyl acetate                        | 223.0                  | 18                | 82                 |
| Ethyl fumarate                        | 217.1                  | 10                | 90                 |
| Dimethyl <i>o</i> -phthalate          | 245.4                  | 96.3              | 3.7                |
| Methyl salicylate                     | 220.6                  | 15                | 85                 |
| 2-Hydroxy-1-isopropyl-4-methylbenzene | 232.3                  | 13                | 87                 |
| 1,2-Dihydroxybenzene                  | 259.5                  | 46                | 54                 |
| Safrole                               | 225.5                  | 33                | 67                 |
| Isosafrole                            | 233.5                  | 46                | 54                 |
| Benzyl phenyl ether                   | 241.5                  | 80                | 20                 |
| Nitrobenzene                          | 210.0                  | 10                | 90                 |
| <i>m</i> -Nitrotoluene                | 224.2                  | 25                | 75                 |
| <i>o</i> -Nitrophenol                 | 216.0                  | 10.5              | 89.5               |
| Quinoline                             | 233.6                  | 29                | 71                 |
| <i>p</i> -Dibromobenzene              | 212.9                  | 13                | 87                 |

**TABLE 5.12** Ternary Azeotropic Mixtures

| A. Ternary azeotropes containing water and alcohols |                           |                   |         |                    |
|-----------------------------------------------------|---------------------------|-------------------|---------|--------------------|
| System                                              | BP of<br>azeotrope,<br>°C | Composition, wt % |         |                    |
|                                                     |                           | Water             | Alcohol | Other<br>component |
| Methanol                                            |                           |                   |         |                    |
| Chloroform                                          | 52.3                      | 1.3               | 8.2     | 90.5               |
| 2-Methyl-1,3-butadiene                              | 30.2                      | 0.6               | 5.4     | 94.0               |
| Methyl chloroacetate                                | 67.9                      | 6.3               | 81.2    | 13.5               |
| Ethanol                                             |                           |                   |         |                    |
| Acetonitrile                                        | 72.9                      | 1                 | 55      | 44                 |
| Acrylonitrile                                       | 69.5                      | 8.7               | 20.3    | 71.0               |
| Benzene                                             | 64.9                      | 7.4               | 18.5    | 74.1               |
| Butylamine                                          | 81.8                      | 7.5               | 42.5    | 50.0               |
| Butyl methyl ether                                  | 62                        | 6.3               | 8.6     | 85.1               |
| Carbon disulfide                                    | 41.3                      | 1.6               | 5.0     | 93.4               |
| Carbon tetrachloride                                | 62                        | 4.5               | 10.0    | 85.5               |
| Chloroform                                          | 55.3                      | 2.3               | 3.5     | 94.2               |
| Crotonaldehyde                                      | 78.0                      | 4.8               | 87.9    | 7.3                |
| Cyclohexane                                         | 62.6                      | 4.8               | 19.7    | 75.5               |
| 1,2-Dichloroethane                                  | 66.7                      | 5                 | 17      | 78                 |
| 1,1-Diethoxyethane                                  | 77.8                      | 11.4              | 27.6    | 61.0               |
| Diethoxymethane                                     | 73.2                      | 12.1              | 18.4    | 69.5               |
| Ethyl acetate                                       | 70.2                      | 9.0               | 8.4     | 82.6               |
| Heptane                                             | 68.8                      | 6.1               | 33.0    | 60.9               |
| Hexane                                              | 56.0                      | 3                 | 12      | 85                 |
| Toluene                                             | 74.4                      | 12                | 37      | 51                 |
| Trichloroethylene                                   | 67.0                      | 5.5               | 16.1    | 78.4               |
| Triethylamine                                       | 74.7                      | 9                 | 13      | 78                 |
| 1-Propanol                                          |                           |                   |         |                    |
| Benzene                                             | 67                        | 7.6               | 10.1    | 82.3               |
| Carbon tetrachloride                                | 65.4                      | 5                 | 11      | 84                 |
| Cyclohexane                                         | 66.6                      | 8.5               | 10.0    | 81.5               |
| 1,1-Dipropoxyethane                                 | 87.6                      | 27.4              | 51.6    | 21.0               |
| Dipropoxymethane                                    | 86.4                      | 8.0               | 44.8    | 47.2               |
| Dipropyl ether                                      | 74.8                      | 11.7              | 20.2    | 68.1               |
| 3-Pentanone                                         | 81.2                      | 20                | 20      | 60                 |
| Propyl acetate                                      | 82.5                      | 17.0              | 10.0    | 73.0               |
| Propyl formate                                      | 70.8                      | 13                | 5       | 82                 |
| Tetrachloroethylene                                 | 81.2                      | 12.5              | 20.7    | 66.8               |
| 2-Propanol                                          |                           |                   |         |                    |
| Benzene                                             | 66.5                      | 7.5               | 18.7    | 73.8               |
| Butylamine                                          | 83                        | 12.5              | 40.5    | 47.0               |

**TABLE 5.12** Ternary Azeotropic Mixtures (*Continued*)

| System                          | BP of<br>azeotrope,<br>°C | Composition, wt % |         |                    |
|---------------------------------|---------------------------|-------------------|---------|--------------------|
|                                 |                           | Water             | Alcohol | Other<br>component |
| 2-Propanol ( <i>continued</i> ) |                           |                   |         |                    |
| Cyclohexane                     | 64.3                      | 7.5               | 18.5    | 74.0               |
| Toluene                         | 76.3                      | 13.1              | 38.2    | 48.7               |
| Trichloroethylene               | 69.4                      | 7                 | 20      | 73                 |
| 1-Butanol                       |                           |                   |         |                    |
| Butyl acetate                   | 89.4                      | 37.3              | 27.4    | 35.3               |
| Butyl formate                   | 83.6                      | 21.3              | 10.0    | 68.7               |
| Dibutyl ether                   | 90.6                      | 29.9              | 34.6    | 35.5               |
| Heptane                         | 78.1                      | 41.4              | 7.6     | 51.0               |
| Hexane                          | 61.5                      | 19.2              | 2.9     | 77.9               |
| Nonane                          | 90.0                      | 69.9              | 18.3    | 11.8               |
| Octane                          | 86.1                      | 60.0              | 14.6    | 25.4               |
| 2-Butanol                       |                           |                   |         |                    |
| Carbon tetrachloride            | 65                        | 4.05              | 4.95    | 91.00              |
| Cyclohexane                     | 69.7                      | 8.9               | 10.8    | 80.3               |
| Isooctane                       | 76.3                      | 9                 | 19      | 72                 |
| 2-Methyl-1-propanol             |                           |                   |         |                    |
| Isobutyl acetate                | 86.8                      | 30.4              | 23.1    | 46.5               |
| Isobutyl formate                | 80.2                      | 17.3              | 6.7     | 76.0               |
| Toluene                         | 81.3                      | 17.9              | 16.4    | 65.7               |
| 2-Methyl-2-propanol             |                           |                   |         |                    |
| Benzene                         | 67.3                      | 8.1               | 21.4    | 70.5               |
| Carbon tetrachloride            | 64.7                      | 3.1               | 11.9    | 85.0               |
| Cyclohexane                     | 65.0                      | 8                 | 21      | 71                 |
| 3-Methyl-1-butanol              |                           |                   |         |                    |
| Isopentyl acetate               | 93.6                      | 44.8              | 31.2    | 24.0               |
| Isopentyl formate               | 89.8                      | 32.4              | 19.6    | 48.0               |
| Allyl alcohol                   |                           |                   |         |                    |
| Benzene                         | 68.2                      | 8.6               | 9.2     | 82.2               |
| Carbon tetrachloride            | 65.2                      | 5                 | 11      | 84                 |
| Cyclohexane                     | 66.2                      | 8                 | 11      | 81                 |
| Hexane                          | 59.7                      | 8.5               | 5.1     | 86.4               |

**TABLE 5.12** Ternary Azeotropic Mixtures (*Continued*)

| <i>B. Other ternary azeotropes</i> |                        |                      |              |                        |                      |
|------------------------------------|------------------------|----------------------|--------------|------------------------|----------------------|
| System                             | BP of<br>azeotrope, °C | Composition,<br>wt % | System       | BP of<br>azeotrope, °C | Composition,<br>wt % |
| Water                              | 32.5                   | 0.4                  | Water        | 71.4                   | 7.9                  |
| Acetone                            |                        | 7.6                  | Nitromethane |                        | 29.7                 |
| 2-Methyl-1,3-butadiene             |                        | 92.0                 | Heptane      |                        | 62.4                 |
| Water                              | 66                     | 8.2                  | Water        | 80.7                   | 17.4                 |
| Acetonitrile                       |                        | 23.3                 | Nitromethane |                        | 58.3                 |
| Benzene                            |                        | 68.5                 | Nonane       |                        | 24.3                 |
| Water                              | 67                     | 6.4                  | Water        | 77.4                   | 12.4                 |
| Acetonitrile                       |                        | 20.5                 | Nitromethane |                        | 44.3                 |
| Trichloroethylene                  |                        | 73.1                 | Octane       |                        | 43.3                 |
| Water                              | 68.6                   | 3.5                  | Water        | 33.1                   | 2.1                  |
| Acetonitrile                       |                        | 9.6                  | Nitromethane |                        | 6.5                  |
| Triethylamine                      |                        | 86.9                 | Pentane      |                        | 91.4                 |
| Water                              | 63.6                   | 5                    | Water        | 82.8                   | 20.6                 |
| 2-Butanone                         |                        | 35                   | Nitromethane |                        | 73.3                 |
| Cyclohexane                        |                        | 60                   | Undecane     |                        | 6.1                  |
| Water                              | 55.0                   | 4                    | Water        | 93.5                   | 40.5                 |
| Butyraldehyde                      |                        | 21                   | Pyridine     |                        | 54.5                 |
| Hexane                             |                        | 75                   | Dodecane     |                        | 5.0                  |
| Water                              | 107.6                  | 21.3                 | Water        | 93.1                   | 38.5                 |
| Formic acid                        |                        | 76.3                 | Pyridine     |                        | 51.0                 |
| Isopentanoic acid                  |                        | 2.4                  | Undecane     |                        | 10.5                 |
| Water                              | 107.0                  | 15.5                 | Water        | 92.3                   | 35.5                 |
| Formic acid                        |                        | 66.8                 | Pyridine     |                        | 45.5                 |
| Isobutyric acid                    |                        | 17.7                 | Decane       |                        | 19.0                 |

**TABLE 5.12** Ternary Azeotropic Mixtures (*Continued*)

| System            | BP of<br>azeotrope, °C | Composition,<br>wt % | System           | BP of<br>azeotrope, °C | Composition,<br>wt % |
|-------------------|------------------------|----------------------|------------------|------------------------|----------------------|
| Water             | 107.6                  | 19.5                 | Water            | 90.5                   | 30.5                 |
| Formic acid       |                        | 75.9                 | Pyridine         |                        | 37.0                 |
| Butyric acid      |                        | 4.6                  | Nonane           |                        | 32.5                 |
| Water             | 107.2                  | 18.6                 | Water            | 86.7                   | 22.4                 |
| Formic acid       |                        | 71.9                 | Pyridine         |                        | 25.5                 |
| Propionic acid    |                        | 9.5                  | Octane           |                        | 52.0                 |
| Water             | 105                    | 11.0                 | Water            | 78.6                   | 14.0                 |
| Hydrogen bromide  |                        | 10.4                 | Pyridine         |                        | 15.5                 |
| Chlorobenzene     |                        | 78.6                 | Heptane          |                        | 70.5                 |
| Water             | 96.9                   | 20.2                 | Acetic acid      | 134.4                  | 23                   |
| Hydrogen chloride |                        | 5.3                  | Pyridine         |                        | 55                   |
| Chlorobenzene     |                        | 74.5                 | Acetic anhydride |                        | 22                   |
| Water             | 107.3                  | 64.8                 | Acetic acid      | 134.1                  | 31.4                 |
| Hydrogen chloride |                        | 15.8                 | Pyridine         |                        | 38.2                 |
| Phenol            |                        | 19.4                 | Decane           |                        | 30.4                 |
| Water             | 116.1                  | 54                   | Acetic acid      | 129.1                  | 13.5                 |
| Hydrogen fluoride |                        | 10                   | Pyridine         |                        | 25.2                 |
| Fluorosilic acid  |                        | 36                   | Ethylbenzene     |                        | 61.3                 |
| Water             | 75.1                   | 11.5                 | Acetic acid      | 98.5                   | 3.4                  |
| Nitroethane       |                        | 75.1                 | Pyridine         |                        | 10.6                 |
| Heptane           |                        | 64.0                 | Heptane          |                        | 86.0                 |
| Water             | 59.5                   | 8.4                  | Acetic acid      | 128.0                  | 20.7                 |
| Nitroethane       |                        | 9.3                  | Pyridine         |                        | 29.4                 |
| Hexane            |                        | 82.3                 | Nonane           |                        | 49.9                 |
| Water             | 82.4                   | 19.1                 | Acetic acid      | 115.7                  | 10.4                 |
| Nitromethane      |                        | 68.1                 | Pyridine         |                        | 20.1                 |
| Decane            |                        | 12.8                 | Octane           |                        | 69.5                 |

**TABLE 5.12** Ternary Azeotropic Mixtures (*Continued*)

| System               | BP of<br>azeotrope, °C | Composition,<br>wt % | System           | BP of<br>azeotrope, °C | Composition,<br>wt % |
|----------------------|------------------------|----------------------|------------------|------------------------|----------------------|
| Water                | 83.1                   | 21.5                 | Acetic acid      | 132.2                  | 17.7                 |
| Nitromethane         |                        | 75.3                 | Pyridine         |                        | 30.5                 |
| Dodecane             |                        | 3.2                  | <i>o</i> -Xylene |                        | 51.8                 |
| Acetic acid          | 129.2                  | 10.2                 | Methanol         | 47.4                   | 14.6                 |
| Pyridine             |                        | 22.5                 | Methyl acetate   |                        | 36.8                 |
| <i>p</i> -Xylene     |                        | 67.3                 | Hexane           |                        | 48.6                 |
| Acetic acid          | 163.0                  | 75.0                 | Ethanol          | 63.2                   | 10.4                 |
| 2,6-Dimethylpyridine |                        | 13.8                 | Acetone          |                        | 24.3                 |
| Undecane             |                        | 11.2                 | Chloroform       |                        | 65.3                 |
| Acetic acid          | 147.0                  | 12.6                 | Ethanol          | 70.1                   | 8                    |
| 2,6-Dimethylpyridine |                        | 74.3                 | Acetonitrile     |                        | 34                   |
| Decane               |                        | 13.1                 | Triethylamine    |                        | 58                   |
| Acetic acid          | 141.3                  | 19.9                 | Ethanol          | 64.7                   | 29.6                 |
| 2-Methylpyridine     |                        | 46.8                 | Benzene          |                        | 12.8                 |
| Decane               |                        | 33.3                 | Cyclohexane      |                        | 57.6                 |
| Acetic acid          | 135.0                  | 12.8                 | Ethanol          | 57.3                   | 9.5                  |
| 2-Methylpyridine     |                        | 38.4                 | Chloroform       |                        | 56.1                 |
| Nonane               |                        | 48.8                 | Hexane           |                        | 34.4                 |
| Acetic acid          | 121.3                  | 3.6                  | 1-Propanol       | 73.8                   | 15.5                 |
| 2-Methylpyridine     |                        | 24.8                 | Benzene          |                        | 30.4                 |
| Octane               |                        | 71.6                 | Cyclohexane      |                        | 54.2                 |
| Acetic acid          | 77.2                   | 7.6                  | 2-Propanol       | 69.1                   | 31.1                 |
| Benzene              |                        | 34.4                 | Benzene          |                        | 15.0                 |
| Cyclohexane          |                        | 58.0                 | Cyclohexane      |                        | 53.9                 |
| Acetic acid          | 132                    | 15                   | 1-Butanol        | 77.4                   | 4                    |
| 2-Methyl-1-butanol   |                        | 54                   | Benzene          |                        | 48                   |
| Isopentyl acetate    |                        | 31                   | Cyclohexane      |                        | 48                   |
| Propionic acid       | 149.3                  | 29.5                 | 1-Butanol        | 108.7                  | 11.9                 |
| 2-Methylpyridine     |                        | 32.0                 | Pyridine         |                        | 20.7                 |
| Decane               |                        | 38.5                 | Toluene          |                        | 76.4                 |

**TABLE 5.12** Ternary Azeotropic Mixtures (*Continued*)

| System           | BP of<br>azeotrope, °C | Composition,<br>wt % | System                  | BP of<br>azeotrope, °C | Composition,<br>wt % |
|------------------|------------------------|----------------------|-------------------------|------------------------|----------------------|
| Propionic acid   | 140.1                  | 16.5                 | 1,2-Ethanediol          | 185.0                  | 8.7                  |
| 2-Methylpyridine |                        | 21.5                 | Phenol                  |                        | 74.6                 |
| Nonane           |                        | 42.0                 | 2,6-Dimethylpyridine    |                        | 16.7                 |
| Propionic acid   | 123.7                  | 4.5                  | 1,2-Ethanediol          | 185.1                  | 5.9                  |
| 2-Methylpyridine |                        | 10.5                 | Phenol                  |                        | 79.1                 |
| Octane           |                        | 85.0                 | 2-Methylpyridine        |                        | 15.0                 |
| Propionic acid   | 153.4                  | 43.0                 | 1,2,-Ethanediol         | 186.4                  | 15.9                 |
| 2-Methylpyridine |                        | 40.0                 | Phenol                  |                        | 67.7                 |
| Undecane         |                        | 17.0                 | 3-Methylpyridine        |                        | 16.4                 |
| Propionic acid   | 147.1                  | 55.5                 | 1,2-Ethanediol          | 188.6                  | 29.5                 |
| Pyridine         |                        | 26.4                 | Phenol                  |                        | 54.8                 |
| Undecane         |                        | 18.1                 | 2,4,6-Trimethylpyridine |                        | 15.7                 |
| Methanol         | 57.5                   | 23                   | Acetone                 | 60.8                   | 3.6                  |
| Acetone          |                        | 30                   | Chloroform              |                        | 68.8                 |
| Chloroform       |                        | 47                   | Hexane                  |                        | 27.6                 |
| Methanol         | 47                     | 14.6                 | Acetone                 | 49.7                   | 51.1                 |
| Acetone          |                        | 30.8                 | Methyl acetate          |                        | 5.6                  |
| Hexane           |                        | 59.6                 | Hexane                  |                        | 43.3                 |
| Methanol         | 53.7                   | 17.4                 | Chloroform              | 62.0                   | 79.7                 |
| Acetone          |                        | 5.8                  | Ethyl formate           |                        | 5.3                  |
| Methyl acetate   |                        | 76.8                 | 2-Bromopropane          |                        | 15.7                 |
| Methanol         | 50.8                   | 17.8                 | 1,4-Dioxane             | 101.8                  | 44.3                 |
| Methyl acetate   |                        | 48.6                 | 2-Methyl-1-propanol     |                        | 26.7                 |
| Cyclohexane      |                        | 33.6                 | Toluene                 |                        | 29.0                 |

5.4 FREEZING MIXTURES

TABLE 5.13 Compositions of Aqueous Antifreeze Solutions

| Freezing point of ethyl alcohol-water mixtures* |                        |                        |                |       |
|-------------------------------------------------|------------------------|------------------------|----------------|-------|
| Specific gravity<br>20°/4°C. (68°F.)            | % alcohol<br>by weight | % alcohol<br>by volume | Freezing point |       |
|                                                 |                        |                        | °C.            | °F.   |
| 0.99363                                         | 2.5                    | 3.13                   | −1.0           | 30.2  |
| 0.98971                                         | 4.8                    | 6.00                   | −2.0           | 28.4  |
| 0.98658                                         | 6.8                    | 8.47                   | −3.0           | 26.6  |
| 0.98006                                         | 11.3                   | 14.0                   | −5.0           | 23.0  |
| 0.97670                                         | 13.8                   | 17.0                   | −6.1           | 21.0  |
| 0.97336                                         | 16.4                   | 20.2                   | −7.5           | 18.5  |
| 0.97194                                         | 17.5                   | 21.5                   | −8.7           | 16.3  |
| 0.97024                                         | 18.8                   | 23.1                   | −9.4           | 15.1  |
| 0.96823                                         | 20.3                   | 24.8                   | −10.6          | 12.9  |
| 0.96578                                         | 22.1                   | 27.0                   | −12.2          | 10.0  |
| 0.96283                                         | 24.2                   | 29.5                   | −14.0          | 6.8   |
| 0.95914                                         | 26.7                   | 32.4                   | −16.0          | 3.2   |
| 0.95400                                         | 29.9                   | 36.1                   | −18.9          | −2.0  |
| 0.94715                                         | 33.8                   | 40.5                   | −23.6          | −10.5 |
| 0.93720                                         | 39.0                   | 46.3                   | −28.7          | −19.7 |
| 0.92193                                         | 46.3                   | 53.8                   | −33.9          | −29.0 |
| 0.90008                                         | 56.1                   | 63.6                   | −41.0          | −41.8 |
| 0.86311                                         | 71.9                   | 78.2                   | −51.3          | −60.3 |

Freezing point of methyl (wood) alcohol-water mixtures\*

| Specific gravity<br>15.6°C. (60°F.) | % alcohol<br>by weight | % alcohol<br>by volume | Freezing point |     |
|-------------------------------------|------------------------|------------------------|----------------|-----|
|                                     |                        |                        | °C.            | °F. |
| 0.993                               | 3.9                    | 5                      | −2.2           | 28  |
| 0.986                               | 8.1                    | 10                     | −5.0           | 23  |
| 0.980                               | 12.2                   | 15                     | −8.3           | 17  |
| 0.974                               | 16.4                   | 20                     | −11.7          | 11  |
| 0.968                               | 20.6                   | 25                     | −15.6          | 4   |
| 0.963                               | 24.9                   | 30                     | −20.0          | −4  |
| 0.956                               | 29.2                   | 35                     | −25.0          | −13 |
| 0.949                               | 33.6                   | 40                     | −30.0          | −22 |
| 0.942                               | 38.0                   | 45                     | −35.6          | −32 |

\* Values are for pure alcohol. Since some commercial antifreezes contain small amounts of water, slightly higher volume concentrations than those given in the table may be required. Antifreezes also contain corrosion inhibitors and other additives to make them function properly as cooling liquids. These affect freezing point slightly and specific gravity to a greater degree. If a protection table is furnished by the manufacturer it should be used in preference to the values given above for the pure substance.



**TABLE 5.13** Compositions of Aqueous Antifreeze Solutions (*Continued*)

| Freezing point of Prestone-water mixtures† |           |                  |                |        |
|--------------------------------------------|-----------|------------------|----------------|--------|
| % Prestone                                 |           | Specific gravity | Freezing point |        |
| By weight                                  | By volume | 15°/15C. (59°F.) | °C.            | °F.    |
| 10                                         | 9.2       | 1.013            | − 3.6          | 25.6   |
| 15                                         | 13.8      | 1.019            | − 5.6          | 22.0   |
| 20                                         | 18.3      | 1.026            | − 7.9          | 17.8   |
| 25                                         | 23.0      | 1.033            | − 10.7         | 12.8   |
| 30                                         | 28.0      | 1.040            | − 14.0         | 6.8    |
| 40                                         | 37.8      | 1.053            | − 22.3         | − 8.2  |
| 50                                         | 47.8      | 1.067            | − 33.8         | − 28.8 |
| 60                                         | 58.1      | 1.079            | − 49.3         | − 56.7 |

Freezing point of ethyl alcohol-water mixtures

| Specific gravity<br>15.6°C. (60°F.) | % alcohol<br>by volume | Freezing point |      |
|-------------------------------------|------------------------|----------------|------|
|                                     |                        | °C.            | °F.  |
| 0.990                               | 5                      | − 1.7          | 29   |
| 0.984                               | 10                     | − 3.3          | 26   |
| 0.978                               | 15                     | − 6.1          | 21   |
| 0.972                               | 20                     | − 8.3          | 17   |
| 0.964                               | 25                     | − 11.1         | 12   |
| 0.955                               | 30                     | − 14.4         | 6    |
| 0.945                               | 35                     | − 17.8         | 0    |
| 0.933                               | 40                     | − 18.3         | − 1  |
| 0.922                               | 45                     | − 18.9         | − 2  |
| 0.910                               | 50                     | − 20.0         | − 4  |
| 0.899                               | 55                     | − 21.7         | − 7  |
| 0.887                               | 60                     | − 23.3         | − 10 |
| 0.875                               | 65                     | − 24.4         | − 12 |
| 0.864                               | 70                     | − 26.7         | − 16 |
| 0.852                               | 75                     | − 32.2         | − 26 |
| 0.840                               | 80                     | − 41.7         | − 43 |

† Eveready Prestone marketed for antifreeze purposes, is 97% ethylene glycol containing fractional percentages of soluble and insoluble ingredients to prevent foaming, creepage and water corrosion in automobile cooling systems.

**TABLE 5.13** Compositions of Aqueous Antifreeze Solutions (*Continued*)

## Freezing point of propylene glycol-water mixtures\*

| Specific gravity<br>15.6°C. (60°F.) | % glycol<br>by volume | Freezing point |      |
|-------------------------------------|-----------------------|----------------|------|
|                                     |                       | °C.            | °F.  |
| 1.004                               | 5                     | − 1.1          | 30   |
| 1.006                               | 10                    | − 2.2          | 28   |
| 1.012                               | 15                    | − 3.9          | 25   |
| 1.017                               | 20                    | − 6.7          | 20   |
| 1.020                               | 25                    | − 8.9          | 16   |
| 1.024                               | 30                    | − 12.8         | 9    |
| 1.028                               | 35                    | − 16.1         | 3    |
| 1.032                               | 40                    | − 20.6         | − 5  |
| 1.037                               | 45                    | − 26.7         | − 16 |
| 1.040                               | 50                    | − 33.3         | − 28 |

## Freezing point of glycerol-water mixtures†

| % Glycerol<br>by weight | Specific gravity<br>15°/15°C. (59°F.) | Specific gravity<br>20°/20°C. (68°F.) | Freezing point |        |
|-------------------------|---------------------------------------|---------------------------------------|----------------|--------|
|                         |                                       |                                       | °C.            | °F.    |
| 10                      | 1.02415                               | 1.02395                               | − 1.6          | 29.1   |
| 20                      | 1.04935                               | 1.04880                               | − 4.8          | 23.4   |
| 30                      | 1.07560                               | 1.07470                               | − 9.5          | 14.9   |
| 40                      | 1.10255                               | 1.10135                               | − 15.5         | 4.3    |
| 50                      | 1.12985                               | 1.12845                               | − 22.0         | − 7.4  |
| 60                      | 1.15770                               | 1.15605                               | − 33.6         | − 28.5 |
| 70                      | 1.18540                               | 1.18355                               | − 37.8         | − 36.0 |
| 80                      | 1.21290                               | 1.21090                               | − 19.2         | − 2.3  |
| 90                      | 1.23950                               | 1.23755                               | − 1.6          | 29.1   |
| 100                     | 1.26557                               | 1.26362                               | 17.0           | 62.6   |

\* Values are for pure alcohol. Since some commercial antifreezes contain small amounts of water, slightly higher volume concentrations than those given in the table may be required. Antifreezes also contain corrosion inhibitors and other additives to make them function properly as cooling liquids. These affect freezing point slightly and specific gravity to a greater degree. If a protection table is furnished by the manufacturer it should be used in preference to the values given above for the pure substance.

† The values are those reported by Bosart and Snoddy (*Jour. Ind. Eng. Chem.*, **19**, 506 (1927)), and Lane (*Jour. Ind. Eng. Chem.*, **17**, 924 (1925)) but modified by adding 2°F to all temperatures below 0°F in accordance with the suggestion of the Procter and Gamble Co.

**TABLE 5.13** Compositions of Aqueous Antifreeze Solutions (*Continued*)

| Freezing point of magnesium chloride brines |                                |                |       |                                  |                                |                |        |
|---------------------------------------------|--------------------------------|----------------|-------|----------------------------------|--------------------------------|----------------|--------|
| % MgCl <sub>2</sub><br>by weight            | Spec. grav.<br>15.6°C. (60°F.) | Freezing point |       | % MgCl <sub>2</sub><br>by weight | Spec. grav.<br>15.6°C. (60°F.) | Freezing point |        |
|                                             |                                | °C.            | °F.   |                                  |                                | °C.            | °F.    |
| 5                                           | 1.043                          | − 3.11         | 26.4  | 18                               | 1.161                          | − 22.1         | − 7.7  |
| 6                                           | 1.051                          | − 3.89         | 25.0  | 19                               | 1.170                          | − 25.6         | − 12.2 |
| 7                                           | 1.060                          | − 4.72         | 23.5  | 20                               | 1.180                          | − 27.4         | − 17.3 |
| 8                                           | 1.069                          | − 5.67         | 21.8  | 21                               | 1.190                          | − 30.6         | − 23.0 |
| 9                                           | 1.078                          | − 6.67         | 20.0  | 22                               | 1.200                          | − 32.8         | − 27.0 |
| 10                                          | 1.086                          | − 7.83         | 17.9  | 23                               | 1.210                          | − 28.9         | − 20.0 |
| 11                                          | 1.096                          | − 9.05         | 15.7  | 24                               | 1.220                          | − 25.6         | − 14.0 |
| 12                                          | 1.105                          | − 10.5         | 13.1  | 25                               | 1.230                          | − 23.3         | − 10.0 |
| 13                                          | 1.114                          | − 12.1         | 10.3  | 26                               | 1.241                          | − 21.1         | − 6.0  |
| 14                                          | 1.123                          | − 13.7         | 7.3   | 27                               | 1.251                          | − 19.4         | − 3.0  |
| 15                                          | 1.132                          | − 15.6         | 4.0   | 28                               | 1.262                          | − 18.3         | − 1.0  |
| 16                                          | 1.142                          | − 17.6         | 0.4   | 29                               | 1.273                          | − 17.2         | + 1.0  |
| 17                                          | 1.151                          | − 19.7         | − 3.5 | 30                               | 1.283                          | − 16.7         | 2.0    |

Freezing point of sodium chloride brines  
Compiled in collaboration with C. D. Looker, Ph.D., International Salt Co., Inc.

| % NaCl<br>by weight | Spec. grav.<br>15°C. (59°F.) | Freezing point |      | % NaCl<br>by weight | Spec. grav.<br>15°C. (59°F.) | Freezing point |        |
|---------------------|------------------------------|----------------|------|---------------------|------------------------------|----------------|--------|
|                     |                              | °C.            | °F.  |                     |                              | °C.            | °F.    |
| 0                   | 1.000                        | 0.00           | 32.0 | 15                  | 1.112                        | − 10.88        | 12.4   |
| 1                   | 1.007                        | − 0.58         | 31.0 | 16                  | 1.119                        | − 11.90        | 10.6   |
| 2                   | 1.014                        | − 1.13         | 30.0 | 17                  | 1.127                        | − 12.93        | 8.7    |
| 3                   | 1.021                        | − 1.72         | 28.9 | 18                  | 1.135                        | − 14.03        | 6.7    |
| 4                   | 1.028                        | − 2.35         | 27.8 | 19                  | 1.143                        | − 15.21        | 4.6    |
| 5                   | 1.036                        | − 2.97         | 26.7 | 20                  | 1.152                        | − 16.46        | 2.4    |
| 6                   | 1.043                        | − 3.63         | 25.5 | 21                  | 1.159                        | − 17.78        | + 0.0  |
| 7                   | 1.051                        | − 4.32         | 24.2 | 22                  | 1.168                        | − 19.19        | − 2.5  |
| 8                   | 1.059                        | − 5.03         | 22.9 | 23                  | 1.176                        | − 20.69        | − 5.2  |
| 9                   | 1.067                        | − 5.77         | 21.6 | 23.3 (E)            | 1.179                        | − 21.13        | − 6.0  |
| 10                  | 1.074                        | − 6.54         | 20.2 | 24                  | 1.184                        | − 17.0*        | + 1.4* |
| 11                  | 1.082                        | − 7.34         | 18.8 | 25                  | 1.193                        | − 10.4*        | 13.3*  |
| 12                  | 1.089                        | − 8.17         | 17.3 | 26                  | 1.201                        | − 2.3*         | 27.9*  |
| 13                  | 1.097                        | − 9.03         | 15.7 | 26.3                | 1.203                        | 0.0*           | 32.0*  |
| 14                  | 1.104                        | − 9.94         | 14.1 |                     |                              |                |        |

\* Saturation temperatures of sodium chloride dihydrate; at these temperatures NaCl · 2H<sub>2</sub>O separates leaving the brine of the eutectic composition (E).

5.4.1 Propylene Glycol–Glycerol

Propylene glycol, a satisfactory antifreeze with the advantage of being nontoxic, can be combined with glycerol, also an efficient nontoxic antifreeze, to give a mixture that can be tested for freezing point with an ethylene glycol (Prestone) hydrometer. A mixture of 70% propylene glycol and 30% glycerol (% by weight of water-free materials), when diluted, can be tested on the standard instrument used for ethylene glycol solutions.

5.5 DENSITY AND SPECIFIC GRAVITY

TABLE 5.14 Density of Mercury and Water

The density of mercury and pure air-free water under a pressure of 101 325 Pa(1 atm) is given in units of grams per cubic centimeter ( $\text{g} \cdot \text{cm}^{-3}$ ). For mercury, the values are based on the density at 20°C being  $13.545\,884\,\text{g} \cdot \text{cm}^{-3}$ . Water attains its maximum density of  $0.999\,973\,\text{g} \cdot \text{cm}^{-3}$  at 3.98°C. For water, the temperature ( $t_m$ , °C) of maximum density at different pressures ( $p$ ) in atmospheres is given by

$$t_m = 3.98 - 0.0225(p - 1)$$

| Density<br>of water | Temp.,<br>°C | Density<br>of mercury | Density<br>of water | Temp.,<br>°C | Density<br>of mercury |
|---------------------|--------------|-----------------------|---------------------|--------------|-----------------------|
|                     | − 20         | 13.644 59             | 0.987 12            | 52           | 13.467 68             |
|                     | − 18         | 13.639 62             | 0.986 18            | 54           | 13.462 82             |
|                     | − 16         | 13.634 66             | 0.985 21            | 56           | 13.457 96             |
|                     | − 14         | 13.629 70             | 0.984 22            | 58           | 13.453 09             |
|                     | − 12         | 13.624 75             | 0.983 20            | 60           | 13.448 23             |
|                     | − 10         | 13.619 79             | 0.982 16            | 62           | 13.443 37             |
|                     | − 8          | 13.614 85             | 0.981 09            | 64           | 13.438 52             |
|                     | − 6          | 13.609 90             | 0.980 01            | 66           | 13.433 67             |
|                     | − 4          | 13.604 96             | 0.978 90            | 68           | 13.428 82             |
|                     | − 2          | 13.600 02             | 0.977 77            | 70           | 13.423 97             |
| 0.999 84            | 0            | 13.595 08             | 0.976 61            | 72           | 13.419 13             |
| 0.999 94            | 2            | 13.590 15             | 0.975 44            | 74           | 13.414 28             |
| 0.999 97            | 4            | 13.585 22             | 0.974 24            | 76           | 13.409 43             |
| 0.999 94            | 6            | 13.580 29             | 0.973 03            | 78           | 13.404 60             |
| 0.999 85            | 8            | 13.575 36             | 0.971 79            | 80           | 13.399 77             |
| 0.999 70            | 10           | 13.570 44             | 0.970 53            | 82           | 13.394 92             |
| 0.999 50            | 12           | 13.565 52             | 0.969 26            | 84           | 13.390 09             |
| 0.999 24            | 14           | 13.560 60             | 0.967 96            | 86           | 13.385 26             |
| 0.998 94            | 16           | 13.555 70             | 0.966 65            | 88           | 13.380 42             |
| 0.998 60            | 18           | 13.550 79             | 0.965 31            | 90           | 13.375 60             |
| 0.998 20            | 20           | 13.545 88             | 0.963 96            | 92           | 13.370 77             |
| 0.997 77            | 22           | 13.540 97             | 0.962 59            | 94           | 13.365 94             |
| 0.997 30            | 24           | 13.536 06             | 0.961 20            | 96           | 13.361 12             |
| 0.996 78            | 26           | 13.531 17             | 0.959 79            | 98           | 13.356 30             |
| 0.996 23            | 28           | 13.526 26             | 0.958 36            | 100          | 13.351 48             |
| 0.995 65            | 30           | 13.521 37             |                     | 120          | 13.303 4              |
| 0.995 03            | 32           | 13.516 47             |                     | 140          | 13.255 4              |
| 0.994 37            | 34           | 13.511 58             |                     | 160          | 13.207 6              |
| 0.993 69            | 36           | 13.506 70             |                     | 180          | 13.159 8              |
| 0.992 97            | 38           | 13.501 82             |                     | 200          | 13.112 0              |
| 0.992 22            | 40           | 13.496 93             |                     | 220          | 13.064 5              |
| 0.991 44            | 42           | 13.492 07             |                     | 240          | 13.016 9              |
| 0.990 63            | 44           | 13.487 18             |                     | 260          | 12.969 2              |
| 0.989 79            | 46           | 13.482 29             |                     | 280          | 12.921 5              |
| 0.988 93            | 48           | 13.477 42             |                     | 300          | 12.873 7              |
| 0.988 04            | 50           | 13.472 56             |                     |              |                       |

**TABLE 5.15** Specific Gravity of Air at Various Temperatures

The table below gives the weight in grams  $\times 10^4$  of 1 mL of air at 760 mm of mercury pressure and at the temperature indicated. Density in grams per milliliter is the same as the specific gravity referred to water at 4°C as unity. To convert to density referred to air at 70°F as unity, divide the values below by 12.00.

| t°C. | Sp.Gr. $\times 10^4$ | t°C. | Sp.Gr. $\times 10^4$ | t°C. | Sp.Gr. $\times 10^4$ | t°C. | Sp.Gr. $\times 10^4$ |
|------|----------------------|------|----------------------|------|----------------------|------|----------------------|
| −25  | 14.240               | 15   | 12.255               | 60   | 10.596               | 140  | 8.541                |
| −24  | 14.182               | 16   | 12.213               | 62   | 10.532               | 142  | 8.500                |
| −23  | 14.125               | 17   | 12.170               | 64   | 10.470               | 144  | 8.459                |
| −22  | 14.069               | 18   | 12.129               | 66   | 10.408               | 146  | 8.419                |
| −21  | 14.013               | 19   | 12.087               | 68   | 10.347               | 148  | 8.379                |
| −20  | 13.957               | 20   | 12.046               | 70   | 10.286               | 150  | 8.339                |
| −19  | 13.902               | 21   | 12.004               | 72   | 10.227               | 155  | 8.242                |
| −18  | 13.847               | 22   | 11.964               | 74   | 10.168               | 160  | 8.147                |
| −17  | 13.793               | 23   | 11.923               | 76   | 10.109               | 165  | 8.054                |
| −16  | 13.739               | 24   | 11.883               | 78   | 10.052               | 170  | 7.963                |
| −15  | 13.685               | 25   | 11.843               | 80   | 9.995                | 175  | 7.874                |
| −14  | 13.632               | 26   | 11.803               | 82   | 9.938                | 180  | 7.787                |
| −13  | 13.580               | 27   | 11.764               | 84   | 9.882                | 185  | 7.702                |
| −12  | 13.527               | 28   | 11.725               | 86   | 9.828                | 190  | 7.619                |
| −11  | 13.476               | 29   | 11.686               | 88   | 9.773                | 195  | 7.537                |
| −10  | 13.424               | 30   | 11.647               | 90   | 9.719                | 200  | 7.457                |
| −9   | 13.373               | 31   | 11.609               | 92   | 9.666                | 205  | 7.379                |
| −8   | 13.322               | 32   | 11.570               | 94   | 9.613                | 210  | 7.303                |
| −7   | 13.272               | 33   | 11.533               | 96   | 9.561                | 215  | 7.228                |
| −6   | 13.222               | 34   | 11.495               | 98   | 9.509                | 220  | 7.155                |
| −5   | 13.173               | 35   | 11.458               | 100  | 9.458                | 230  | 7.013                |
| −4   | 13.124               | 36   | 11.420               | 102  | 9.408                | 240  | 6.881                |
| −3   | 13.075               | 37   | 11.383               | 104  | 9.358                | 250  | 6.753                |
| −2   | 13.026               | 38   | 11.347               | 106  | 9.308                | 260  | 6.624                |
| −1   | 12.978               | 39   | 11.310               | 108  | 9.259                | 270  | 6.504                |
| 0    | 12.931               | 40   | 11.274               | 110  | 9.211                | 280  | 6.389                |
| +1   | 12.883               | 41   | 11.238               | 112  | 9.163                | 290  | 6.277                |
| 2    | 12.836               | 42   | 11.202               | 114  | 9.116                | 300  | 6.166                |
| 3    | 12.790               | 43   | 11.167               | 116  | 9.069                | 310  | 6.062                |
| 4    | 12.743               | 44   | 11.132               | 118  | 9.022                | 320  | 5.942                |
| 5    | 12.697               | 45   | 11.097               | 120  | 8.976                | 330  | 5.847                |
| 6    | 12.652               | 46   | 11.062               | 122  | 8.931                | 340  | 5.755                |
| 7    | 12.606               | 47   | 11.027               | 124  | 8.886                | 350  | 5.664                |
| 8    | 12.561               | 48   | 10.993               | 126  | 8.841                | 360  | 5.578                |
| 9    | 12.517               | 49   | 10.958               | 128  | 8.797                | 370  | 5.493                |
| 10   | 12.472               | 50   | 10.924               | 130  | 8.753                | 380  | 5.407                |
| 11   | 12.428               | 52   | 10.857               | 132  | 8.710                | 400  | 5.248                |
| 12   | 12.385               | 54   | 10.791               | 134  | 8.667                | 420  | 5.101                |
| 13   | 12.341               | 56   | 10.725               | 136  | 8.625                | 440  | 4.952                |
| 14   | 12.298               | 58   | 10.660               | 138  | 8.583                | 460  | 4.812                |

**5.5.1 Density of Moist Air**

The density of moist air depends upon the temperature, the humidity, and the barometric pressure. It is expressed by the equation

$$d_t = D_t \times \frac{P - 0.3783e}{760}$$

where  $d_t$  is the density of the moist air at the temperature  $t$ ;  $D_t$  is the density of dry air at the temperature  $t$  (see Table 5.15, Specific Gravity of Air at Various Temperatures);  $P$  is the height of the barometer after correction and reduction to standard conditions, and is expressed in millimeters of mercury (see Sec. 2.1.3, Barometry and Barometric Corrections);  $e$  is the vapor pressure of water at the temperature of the dew point and is expressed in millimeters of mercury (see Table 5.6, Vapor Pressure of Water).

*Example.* To find the density of moist air at a temperature of 20°C, with a dew point of 10°C, and a corrected barometric pressure of 750 mm.

Reference to Table 5.15 shows that  $D$  at 20°C is equal to 0.001 204 6 g/mL. Reference to Table 5.6 shows that at 10°C (the temperature of the dew point)  $e$  is equal to 9.209 mm. Therefore,

$$\begin{aligned} d &= 0.001\,204\,6 \times \frac{750 - (0.3783 \times 9.209)}{760} \\ &= 0.001\,183\,2 \text{ g/mL} = 1.1832 \text{ g/L} \end{aligned}$$

## 5.5.2 Specific Gravity Corrections for the Buoyant Effect of Air

### 5.5.2.1 Determinations Made with a Pycnometer

$$\begin{aligned} D_{\text{vac}} &= \frac{W_2}{W_1} d - 0.0012 \left( \frac{W_2 d}{W_1} - 1 \right) \\ S_{\text{vac}} &= \frac{W_2}{W_1} - 0.0012 \left( \frac{W_2}{W_1} - 1 \right) \end{aligned}$$

where  $D_{\text{vac}}$  = density of the liquid in grams per milliliter at  $t^\circ\text{C}$  corrected for the buoyant effect of air

$W_1$  = weight in air of the water required to fill the pycnometer at  $t^\circ\text{C}$

$W_2$  = weight in air of the liquid required to fill the pycnometer at  $t^\circ\text{C}$

$d$  = density of water in grams per milliliter at  $t^\circ\text{C}$

$S_{\text{vac}}$  = specific gravity of the liquid at  $t^\circ\text{C}$  referred to water at  $t^\circ\text{C}$  corrected for the buoyant effect of air

When the weight of the water is determined at a temperature of  $t^\circ\text{C}$ , and that of the liquid at a different temperature  $t'$ , the equations above are modified as follows:

$$\begin{aligned} D_{\text{vac}} &= \frac{W_2}{W_1} d - 0.0012 \left( \frac{W_2}{W_1} d - 1 \right) + 0.000\,026 (t' - t^\circ) \left( \frac{W_2}{W_1} d \right) \\ S_{\text{vac}} &= \frac{W_2}{W_1} - 0.0012 \left( \frac{W_2}{W_1} - 1 \right) + 0.000\,026 (t' - t^\circ) \left( \frac{W_2}{W_1} \right) \end{aligned}$$

**5.5.2.2 Determinations Made with a Plummet or Sinkers.** The equations above may also be used when the density is determined with plummet or sinker, but in this case

$W_1$  = weight of the plummet in air minus its weight in water

$W_2$  = weight of the plummet in air minus its weight in the liquid

5.6 VISCOSITY, SURFACE TENSION, DIELECTRIC CONSTANT, DIPOLE MOMENT, AND REFRACTIVE INDEX

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances

For the majority of substances the dependence of the surface tension  $\gamma$  on the temperature can be given as:

$$\gamma = a - bt$$

where  $a$  and  $b$  are constants and  $t$  is the temperature in degrees Celsius. In the SI system the surface tensions are expressed in  $\text{mN} \cdot \text{m}^{-1}$  ( $= \text{dyn} \cdot \text{cm}^{-1}$ ).

A compilation of some 2200 liquid compounds has been prepared by J. J. Jasper, *J. Phys. Chem. Reference Data* 1:841 (1972).

The SI unit of viscosity is pascal-second ( $\text{Pa} \cdot \text{s}$ ) or newton-second per meter squared ( $\text{N} \cdot \text{s} \cdot \text{m}^{-2}$ ). Values tabulated are  $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$  ( $=$  centipoise, cP). The temperature in degrees Celsius at which the viscosity of a substance was measured is shown in parentheses after the value.

| Substance                | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |           | Liquid range, $^{\circ}\text{C}$           | Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|--------------------------|-----------------------------------------------------|-----------|--------------------------------------------|-----------------------------------------------------------|
|                          | $a$                                                 | $b$       |                                            |                                                           |
| Acetaldehyde             | 23.90                                               | 0.1360    | − 123 to 21                                | 0.2797(0), 0.2557(10), 0.22(20)                           |
| Acetaldoxime             | 34.23                                               | 0.1134    | 12( $\beta$ ) or 46.5( $\alpha$ ) to 114.5 |                                                           |
| Acetamide                | 47.66                                               | 0.1021    | 81 to 222                                  | 1.63(94), 1.32(105), 1.06(120)                            |
| Acetanilide              | 46.21                                               | 0.0912    | 114 to 304                                 | 2.22(120), 1.90(130)                                      |
| Acetic acid              | 29.58                                               | 0.0994    | 16.7 to 118                                | 1.056(25), 0.786(50), 0.424(110)                          |
| Acetic anhydride         | 35.52                                               | 0.1436    | − 73 to 139                                | 1.241(0), 0.907(20), 0.699(40)                            |
| Acetone                  | 26.26                                               | 0.112     | − 94 to 56                                 | 0.395(0), 0.306(25), 0.256(50)                            |
| Acetonitrile             | 29.58                                               | 0.1178    | − 44 to 81.6                               | 0.397(10), 0.329(30), 0.2753(50)                          |
| Acetophenone             | 41.92                                               | 0.1154    | 20 to 202                                  | 1.511(30), 1.192(45), 0.634(100)                          |
| Acetyl chloride          | 26.7(15)                                            |           | − 113 to 51                                | 0.368(25), 0.294(50)                                      |
| Acrylic acid             | 28.1(30)                                            |           | 14 to 141                                  |                                                           |
| Acrylonitrile            | 29.58                                               | 0.1178    | − 83.5 to 77.3                             |                                                           |
| Allyl acetate            | 28.73                                               | 0.1186    | up to 104                                  |                                                           |
| Allyl alcohol            | 27.53                                               | 0.0902    | − 129 to 97                                | 1.218(25), 0.759(50), 0.553(70)                           |
| Allylamine               | 27.49                                               | 0.1287    | − 88 to 55                                 |                                                           |
| Allyl isothiocyanate     | 36.76                                               | 0.1074    | − 80 to 152                                |                                                           |
| 2-Aminoethanol           | 51.11                                               | 0.1117    | 10.3 to 171                                |                                                           |
| Aniline                  | 44.83                                               | 0.1085    | − 6 to 186                                 | 3.847(25), 2.029(50), 1.247(75)                           |
| Benzaldehyde             | 40.72                                               | 0.1090    | − 26 to 179                                |                                                           |
| Benzamide                | 47.26                                               | 0.0705    | 129 to 290                                 |                                                           |
| Benzene                  | 28.88(20)                                           | 27.56(30) | 5.5 to 80                                  | 0.649(20), 0.566(30), 0.395(60)                           |
| Benzenesulfonyl chloride | 45.48                                               | 0.1117    | 14.5 to 251                                |                                                           |
| Benzenethiol             | 41.41                                               | 0.1202    | − 14.9 to 169                              |                                                           |
| Benzonitrile             | 41.69                                               | 0.1159    | − 12.7 to 191                              | 1.447(15), 1.111(30), 0.883(50)                           |
| Benzophenone             | 46.31                                               | 0.1128    | 48 to 305                                  |                                                           |
| Benzoyl bromide          | 45.85                                               | 0.1397    | − 24 to 219                                |                                                           |
| Benzoyl chloride         | 41.34                                               | 0.1084    | − 1 to 197                                 |                                                           |
| Benzyl alcohol           | 38.25                                               | 0.1381    | − 15.2 to 205                              | 5.474(25), 2.760(50), 1.618(75)                           |
| Benzylamine              | 42.33                                               | 0.1213    | 10 to 180                                  | 1.624(25), 1.080(50), 0.769(75)                           |
| Benzyl benzoate          | 48.07                                               | 0.1065    | 21 to 323                                  | 8.454(25)                                                 |
| Benzyl chloride          | 39.92                                               | 0.1227    | − 43 to 179                                |                                                           |

**TABLE 5.16** Viscosity and Surface Tension of Various Organic Substances (*Continued*)

| Substance                 | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup>                                                                  |
|---------------------------|------------------------------------------|-----------|------------------|------------------------------------------------------------------------------------------------------|
|                           | <i>a</i>                                 | <i>b</i>  |                  |                                                                                                      |
| Benzyl ethyl ether        | 32.82(20)                                | 29.97(40) | up to 186        | 1.196(15), 0.985(30), 0.385(1423)<br>0.633(20), 0.606(25), 0.471(50)                                 |
| Biphenyl                  | 41.52                                    | 0.0931    | 69 to 256        |                                                                                                      |
| Bis(2-ethoxyethyl) ether  | 29.74                                    | 0.1176    | – 45 to 188      |                                                                                                      |
| Bis(2-hydroxyethyl) ether | 46.97                                    | 0.0880    | – 10.4 to 246    |                                                                                                      |
| Bis(2-methoxyethyl) ether | 32.47                                    | 0.1164    | – 68 to 162      | 0.477(10), 0.374(25)                                                                                 |
| Bromobenzene              | 38.14                                    | 0.1160    | – 30.6 to 156    |                                                                                                      |
| 1-Bromobutane             | 28.71                                    | 0.1126    | – 112.4 to 101.6 |                                                                                                      |
| (±)-2-Bromobutane         | 27.48                                    | 0.1107    | – 112.7 to 91.4  |                                                                                                      |
| Bromochloromethane        | 33.32(20)                                |           | – 88 to 68       |                                                                                                      |
| Bromocyclohexane          | 36.13                                    | 0.1117    | up to 165.8      |                                                                                                      |
| 1-Bromodecane             | 31.26                                    | 0.0856    | – 30 to 240      |                                                                                                      |
| Bromodichloromethane      | 35.11                                    | 0.1294    | – 55 to 87       |                                                                                                      |
| 1-Bromododecane           | 32.58                                    | 0.0882    | – 11 to bp       |                                                                                                      |
| Bromoethane               | 26.52                                    | 0.1159    | – 119 to 38.2    |                                                                                                      |
| Bromoform                 | 48.14                                    | 0.1308    | 8 to 149         | 0.539(15), 0.459(30), 0.338(70)<br>0.536(15), 0.437(30), 0.359(50)<br>0.620(0), 0.471(25), 0.373(50) |
| 1-Bromoheptane            | 30.74                                    | 0.0982    | – 58 to 180      |                                                                                                      |
| 1-Bromohexadecane         | 33.37                                    | 0.0861    | 17.8 to 336      |                                                                                                      |
| 1-Bromohexane             | 29.81                                    | 0.0967    | – 85 to 158      |                                                                                                      |
| Bromomethane              | 26.52                                    | 0.1159    | – 94 to 3.56     |                                                                                                      |
| 1-Bromo-3-methylbutane    | 28.10                                    | 0.0996    | – 112 to 119.7   |                                                                                                      |
| 1-Bromo-2-methylpropane   | 26.96                                    | 0.1059    | – 119 to 91.5    |                                                                                                      |
| 1-Bromonaphthalene        | 46.44                                    | 0.1018    | – 1.8 to 281     |                                                                                                      |
| 1-Bromononane             | 31.36                                    | 0.0894    | ca. – 55 to 201  |                                                                                                      |
| 1-Bromooctane             | 31.00                                    | 0.0928    | – 55 to 201      |                                                                                                      |
| 1-Bromopentane            | 29.51                                    | 0.1049    | – 88 to 129.6    | 0.553(25), 0.418(50), 0.330(75)                                                                      |
| <i>p</i> -Bromophenol     | 48.88                                    | 0.1070    | 64 to 238        |                                                                                                      |
| 1-Bromopropane            | 28.30                                    | 0.1218    | – 110.1 to 71    |                                                                                                      |
| 2-Bromopropane            | 26.21                                    | 0.1183    | – 89 to 59.5     |                                                                                                      |
| 3-Bromopropene            | 29.45                                    | 0.1257    | – 119 to 70      |                                                                                                      |
| 1-Bromotetradecane        | 32.93                                    | 0.0878    | 6 to > 178       |                                                                                                      |
| <i>o</i> -Bromotoluene    | 36.62                                    | 0.0998    | – 26 to 181      |                                                                                                      |
| <i>p</i> -Bromotoluene    | 36.40                                    | 0.0997    | 28.5 to 184      |                                                                                                      |
| 1-Bromoundecane           | 31.94                                    | 0.0861    | – 9 to > 138     |                                                                                                      |
| Butanal                   | 26.67                                    | 0.0925    | – 99 to 74.8     |                                                                                                      |
| Butane                    | 14.87                                    | 0.1206    | – 138.3 to – 0.5 | 0.428(20), 0.349(40), 0.249(75)                                                                      |
| 1,3-Butanediol            | 37.8(25)                                 |           | < – 50 to 207.5  |                                                                                                      |
| 2,3-Butanediol            | 36(25)                                   |           | 25 to 182        |                                                                                                      |
| Butanenitrile             |                                          |           | – 112 to 117.6   |                                                                                                      |
| Butanesulfonyl chloride   | 37.33                                    | 0.0977    |                  | 1.540(20), 0.980(40), 0.323(60)                                                                      |
| 1-Butanethiol             | 28.07                                    | 0.1142    | – 116 to 98.5    |                                                                                                      |
| Butanoic acid             | 28.35                                    | 0.0920    | – 6 to 163.5     |                                                                                                      |
| Butanoic anhydride        | 28.93(20)                                | 28.44(25) | – 66 to 199.5    |                                                                                                      |
| 1-Butanol                 | 27.18                                    | 0.0898    | – 89.5 to 117.7  | 5.185(0), 2.948(20), 1.782(40)<br>3.907(20), 1.332(50), 0.698(75)                                    |
| (±)-2-Butanol             | 23.47(20)                                | 22.62(30) | – 114.7 to 99.5  |                                                                                                      |
| 2-Butanone                | 26.77                                    | 0.1122    | – 86.7 to 79.6   |                                                                                                      |
| 1-Butene                  | 15.19                                    | 0.1323    | – 185 to – 6.5   |                                                                                                      |
| 2-Butene                  | 16.11                                    | 0.1289    | – 106 to 0.9     |                                                                                                      |
| 3-Butenenitrile           | 31.40                                    | 0.1085    | – 87 to 119      |                                                                                                      |
| 2-Butoxyethanol           | 28.18                                    | 0.0816    | – 75 to 168      |                                                                                                      |



TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                      | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup> |
|--------------------------------|------------------------------------------|-----------|------------------|-------------------------------------|
|                                | <i>a</i>                                 | <i>b</i>  |                  |                                     |
| 2-(2-Butoxyethoxy)ethanol      | 30.0(25)                                 |           | − 68.1 to 230.4  |                                     |
| Butyl acetate                  | 27.55                                    | 0.1068    | − 77 to 126      | 0.734(20), 0.688(25), 0.500(50)     |
| (±)- <i>sec</i> -Butyl acetate | 23.33(22)                                | 21.24(42) | − 99 to 112      | 0.676(25), 0.493(50), 0.370(75)     |
| <i>tert</i> -Butyl acetate     | 24.69                                    | 0.1102    | up to 98         |                                     |
| Butylamine                     | 26.24                                    | 0.1122    | − 50 to 77       | 0.830(0), 0.574(25), 0.409(50)      |
| <i>sec</i> -Butylamine         | 23.75                                    | 0.1057    | − 104 to 63      | 0.770(0), 0.571(25), 0.367(50)      |
| <i>tert</i> -Butylamine        | 19.44                                    | 0.1028    | − 66 to 44       |                                     |
| Butylbenzene                   | 31.28                                    | 0.1025    | − 88 to 183      | 1.035(20), 0.683(50), 0.515(75)     |
| <i>sec</i> -Butylbenzene       | 30.48                                    | 0.0979    | − 82.7 to 173    |                                     |
| <i>tert</i> -Butylbenzene      | 30.10                                    | 0.0985    | − 58.1 to 168.5  |                                     |
| Butyl butanoate                | 27.65                                    | 0.0965    | − 91.5 to 166    |                                     |
| Butyl ethyl ether              | 22.75                                    | 0.1049    | − 124 to 92      |                                     |
| Butyl formate                  | 27.08                                    | 0.1026    | − 91.5 to 106    | 0.940(0), 0.691(20), 0.472(50)      |
| Butyl methyl ether             | 22.17                                    | 0.1057    | − 115.5 to 70    |                                     |
| Butyl nitrate                  | 30.35                                    | 0.1126    | up to 133        |                                     |
| Butyl propanoate               | 27.37                                    | 0.0993    | − 89 to 146.8    |                                     |
| 4- <i>tert</i> -Butylpyridine  | 35.48                                    | 0.0951    | ca. − 44 to 197  |                                     |
| Butyl stearate                 | 33.0(25)                                 | 32.7(30)  | 26 to 343        |                                     |
| Butyl vinyl ether              | 21.99(20)                                |           | − 92 to 94.2     |                                     |
| Carbon disulfide               | 35.29                                    | 0.1484    | − 111.6 to 46.5  | 0.429(0), 0.363(20), 0.352(25)      |
| Carbon tetrachloride           | 29.49                                    | 0.1224    | − 23 to 76.7     | 1.321(0), 0.908(25), 0.656(50)      |
| D-(+)-Carvone                  | 36.54                                    | 0.0920    | < 15 to 230      |                                     |
| Chloroacetic acid              | 43.27                                    | 0.1117    | 61 to 189        | 3.15(50), 1.92(75)                  |
| <i>o</i> -Chloroaniline        | 43.41                                    | 0.0904    | − 14 to 208.8    | 3.316(25), 1.913(50), 1.248(75)     |
| <i>p</i> -Chloroaniline        | 48.69                                    | 0.1099    | 72.5 to 232      |                                     |
| Chlorobenzene                  | 35.97                                    | 0.1191    | − 45.3 to 131.7  | 0.799(20), 0.631(40), 0.512(60)     |
| 1-Chlorobutane                 | 25.97                                    | 0.1117    | − 123.1 to 78.4  | 0.556(0), 0.422(25), 0.329(50)      |
| 2-Chlorobutane                 | 24.40                                    | 0.1118    | − 131.3 to 68.2  | 0.439(15)                           |
| Chlorocyclohexane              | 33.90                                    | 0.1101    | − 44 to 142      |                                     |
| 1-Chlorododecane               | 31.56                                    | 0.0904    | − 9 to 116       |                                     |
| 1-Chloro-2,3-epoxypropane      | 39.76                                    | 0.1360    | − 57.2 to 116.1  | 1.03(25)                            |
| Chloroethane                   | 21.18(5)                                 | 20.58(10) | − 139 to 12.3    | 0.416(− 25), 0.319(0), 0.279(10)    |
| 2-Chloroethanol                | 38.9(20)                                 |           | − 67.5 to 128.6  | 3.913(15)                           |
| Chloroform                     | 29.91                                    | 0.1295    | − 63.6 to 61.1   | 0.706(0), 0.596(15), 0.514(30)      |
| 1-Chloroheptane                | 28.94                                    | 0.0961    | − 69 to 161      |                                     |
| 1-Chlorohexane                 | 28.32                                    | 0.1038    |                  |                                     |
| 1-Chloro-3-methylbutane        | 25.51                                    | 0.1076    | − 104 to 99      |                                     |
| 1-Chloro-2-methylpropane       | 24.40                                    | 0.1099    | − 130.3 to 68.9  | 0.462(20), 0.373(40)                |
| 2-Chloro-2-methylpropane       | 20.06(15)                                | 18.35(30) | − 26 to 50.8     | 0.543(15)                           |
| 1-Chloronaphthalene            | 44.12                                    | 0.1035    | − 2.3 to 259     | 2.940(25)                           |
| <i>o</i> -Chloronitrobenzene   | 48.10                                    | 0.1171    | 33 to 246        |                                     |
| <i>m</i> -Chloronitrobenzene   | 49.71                                    | 0.1417    | 44 to 236        |                                     |
| <i>p</i> -Chloronitrobenzene   | 45.84                                    | 0.1046    | 84 to 242        |                                     |
| 1-Chlorooctane                 | 29.64                                    | 0.0961    | − 58 to 182      |                                     |
| 1-Chloropentane                | 27.09                                    | 0.1076    | − 99 to 108      | 0.580(20)                           |
| <i>o</i> -Chlorophenol         | 42.5                                     | 0.1122    | 9.8 to 175       | 3.589(25), 1.835(50), 1.131(75)     |
| <i>m</i> -Chlorophenol         | 43.7                                     | 0.1009    | 33 to 214        | 11.55(25), 4.725(45), 4.041(50)     |
| <i>p</i> -Chlorophenol         | 46.0                                     | 0.1049    | 43 to 220        | 4.99(50)                            |
| 1-Chloropropane                | 24.41                                    | 0.1246    | − 122.8 to 47    | 0.436(0), 0.372(15), 0.318(30)      |

**TABLE 5.16** Viscosity and Surface Tension of Various Organic Substances (*Continued*)

| Substance                          | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |           | Liquid range, °C | Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|------------------------------------|-----------------------------------------------------|-----------|------------------|-----------------------------------------------------------|
|                                    | <i>a</i>                                            | <i>b</i>  |                  |                                                           |
| 2-Chloropropane                    | 21.37                                               | 0.0883    | − 117 to 36      | 0.401(0), 0.335(15), 0.299(30)                            |
| 3-Chloro-1-propene                 | 25.50                                               | 0.0946    | − 134.5 to 45    | 0.347(15)                                                 |
| <i>o</i> -Chlorotoluene            |                                                     |           | − 35.6 to 159    | 1.267(25), 0.883(50), 0.662(75)                           |
| <i>m</i> -Chlorotoluene            |                                                     |           | − 47.8 to 161.8  | 0.964(25), 0.710(50), 0.547(75)                           |
| <i>p</i> -Chlorotoluene            | 34.93                                               | 0.1082    | 7.5 to 162.4     | 0.837(25), 0.621(50), 0.483(75)                           |
| Chlorotrimethylsilane              | 19.51                                               | 0.0875    | − 40 to 57       |                                                           |
| <i>o</i> -Cresol                   | 39.43                                               | 0.1011    | 30 to 191        | 3.035(50), 1.562(75), 0.961(100)                          |
| <i>m</i> -Cresol                   | 38.00                                               | 0.0924    | 12 to 202        | 12.9(25), 4.417(50), 2.093(75)                            |
| <i>p</i> -Cresol                   | 38.58                                               | 0.0962    | 34.8 to 202      | 5.607(45)                                                 |
| Cycloheptanol                      | 35.02                                               | 0.0923    | 2 to 185         |                                                           |
| Cyclohexane                        | 27.62                                               | 0.1188    | 6.6 to 80.7      | 0.980(20), 0.912(25), 0.650(50)                           |
| Cyclohexanol                       | 35.33                                               | 0.0966    | 25.4 to 161      | 57.5(25), 41.07(30), 12.3(50)                             |
| Cyclohexanone                      | 37.67                                               | 0.1242    | − 31 to 155.7    | 2.453(15), 1.803(30), 1.321(50)                           |
| Cyclohexene                        | 29.23                                               | 0.1223    | − 103.5 to 83    | 0.882(0), 0.625(25), 0.467(50)                            |
| Cyclohexylamine                    | 34.19                                               | 0.1188    | − 18 to 134      | 1.079(25), 0.692(50), 0.485(75)                           |
| Cyclooctane                        | 32.02                                               | 0.1090    | 14.8 to 151.1    |                                                           |
| Cyclopentane                       | 25.53                                               | 0.1462    | − 94 to 50       | 0.555(0), 0.413(25), 0.321(50)                            |
| Cyclopentanol                      | 35.04                                               | 0.1011    | − 19 to 140      | 0.439(20)                                                 |
| Cyclopentanone                     | 35.55                                               | 0.1100    | − 51 to 130.6    |                                                           |
| Cyclopentene                       | 25.94                                               | 0.1495    | − 135.1 to 44.2  |                                                           |
| <i>cis</i> -Decahydronaphthalene   | 32.18(20)                                           | 31.01(30) | − 43 to 195.8    | 3.042(25), 1.875(50), 1.271(75)                           |
| <i>trans</i> -Decahydronaphthalene | 29.89(20)                                           | 28.87(30) | − 30.4 to 187.3  | 1.948(25), 1.289(50), 0.917(75)                           |
| Decamethylcyclopentasiloxane       | 19.56                                               | 0.0565    | − 38 to > 101    |                                                           |
| Decamethyltetrasiloxane            | 86.20(25)                                           |           | − 68 to 194      | 1.28(20)                                                  |
| Decane                             | 25.67                                               | 0.0920    | − 29.7 to 174.1  | 1.277(0), 0.838(25), 0.598(50)                            |
| 1-Decanol                          | 30.34                                               | 0.0732    | 6.9 to 232       | 10.9(25), 4.590(50)                                       |
| 1-Decene                           | 25.84                                               | 0.0919    | − 66 to 170.6    | 0.805(20)                                                 |
| Dibenzylamine                      | 43.27                                               | 0.1086    | − 26 to 300      |                                                           |
| Dibenzyl ether                     | 38.2(35)                                            |           | 2 to 298         | 3.711(25)                                                 |
| <i>p</i> -Dibromobenzene           | 41.84                                               | 0.1007    | 87.3 to 220      |                                                           |
| 1,4-Dibromobutane                  | 48.24                                               | 0.1190    | − 20 to 198      |                                                           |
| 1,2-Dibromoethane                  | 42.85                                               | 0.1320    | 10 to 131.7      | 1.721(20), 1.286(40), 0.648(100)                          |
| 1,2-Dibromopropane                 | 36.81                                               | 0.1155    | − 55.5 to 142    | 1.5(25)                                                   |
| Dibromotetrafluoroethane           | 18.9(20)                                            | 18.1(25)  | − 110.5 to 47    | 0.72(25)                                                  |
| Dibutylamine                       | 26.50                                               | 0.0952    | − 62 to 159.6    | 0.918(25), 0.619(50), 0.449(75)                           |
| Dibutyl decanedioate               |                                                     |           | − 10 to 345      | 9.03(25)                                                  |
| Dibutyl ether                      | 24.78                                               | 0.0934    | − 95 to 140      | 0.637(25), 0.466(50), 0.356(75)                           |
| Dibutyl maleate                    | 32.46                                               | 0.0865    | < − 80 to 281    | 5.62(20), 4.76(25)                                        |
| Dibutyl <i>o</i> -phthalate        | 33.40(20)                                           |           | − 35 to 340      | 19.91(20), 11.17(35), 7.85(45)                            |
| Dichloroacetic acid                | 37.8                                                | 0.0927    | 9 to 194         | 3.23(50), 1.92(75)                                        |
| <i>o</i> -Dichlorobenzene          | 35.55(30)                                           |           | − 17 to 180.4    | 1.324(25), 0.962(50), 0.739(75)                           |
| <i>m</i> -Dichlorobenzene          | 38.30                                               | 0.1147    | − 24.8 to 173.1  | 1.044(25), 0.783(50), 0.628(75)                           |
| <i>p</i> -Dichlorobenzene          | 34.66                                               | 0.0879    | 53 to 174.1      | 0.839(55), 0.668(79)                                      |
| 1,4-Dichlorobutane                 | 37.79                                               | 0.1174    | − 38 to 163      |                                                           |
| 1,1-Dichloroethane                 | 27.03                                               | 0.1186    | − 97 to 57.3     | 0.505(15), 0.464(25), 0.362(50)                           |
| 1,2-Dichloroethane                 | 35.43                                               | 0.1428    | − 35.7 to 83.5   | 1.125(0), 0.779(25), 0.576(50)                            |
| 1,1-Dichloroethylene               |                                                     |           | − 122.6 to 31.6  | 0.442(0), 0.358(20)                                       |
| <i>cis</i> -1,2-Dichloroethylene   | 28(20)                                              |           | − 80.1 to 60     | 0.785(− 25), 0.575(0), 0.444(25)                          |
| <i>trans</i> -1,2-Dichloroethylene | 25(20)                                              |           | − 49.8 to 48.7   | 0.522(− 25), 0.398(0), 0.317(25)                          |
| 2,2'-Dichloroethyl ether           | 40.57                                               | 0.1306    | up to 178.5      | 2.41(20), 2.065(25)                                       |

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                               | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup> |
|-----------------------------------------|------------------------------------------|-----------|------------------|-------------------------------------|
|                                         | <i>a</i>                                 | <i>b</i>  |                  |                                     |
| Dichloromethane                         | 30.41                                    | 0.1284    | − 95 to 40       | 0.533(0), 0.449(15), 0.393(30)      |
| 2,4-Dichlorophenol                      | 46.59                                    | 0.1221    | 42 to 210        |                                     |
| 1,2-Dichloropropane                     | 31.42                                    | 0.1240    | − 100 to 96      | 0.865(20), 0.700(25)                |
| 1,3-Dichloropropane                     | 36.40                                    | 0.1233    | − 99.5 to 122    |                                     |
| 2,2-Dichloropropane                     | 23.60(20)                                | 22.53(30) | − 35 to 69       | 0.769(15), 0.619(30)                |
| α,α-Dichlorotoluene                     | 41.26                                    | 0.1035    | − 16 to 205      |                                     |
| Diethanolamine                          |                                          |           | 28 to 269        | 368(30), 109.5(50), 28.7(75)        |
| 1,1-Diethoxyethane                      | 23.46                                    | 0.1030    | − 100 to 102.2   |                                     |
| 1,2-Diethoxyethane                      |                                          |           | − 74 to 121.4    | 0.65(20)                            |
| Dimethoxymethane                        | 23.87                                    | 0.1291    | up to 88         |                                     |
| Diethylamine                            | 22.71                                    | 0.1143    | − 50 to 55.5     |                                     |
| <i>N,N</i> -Diethylaniline              | 36.59                                    | 0.1040    | − 38 to 217      | 3.838(0), 1.15(50), 0.750(75)       |
| Diethyl carbonate                       | 28.62                                    | 0.1100    | − 43 to 126      | 0.868(15), 0.748(25)                |
| Diethyl decanedioate                    | 34.68                                    | 0.0959    |                  |                                     |
| Diethyl ether                           | 18.92                                    | 0.0908    | − 116 to 34.6    | 0.283(0), 0.224(25)                 |
| Diethyl ethyl phosphonate               | 30.63                                    | 0.0975    | up to 198        | 1.627(15), 0.969(45), 0.743(65)     |
| Di(2-ethylhexyl) <i>o</i> -phthalate    |                                          |           | − 50 to 384      | 33.67(35), 21.40(45)                |
| Diethyl maleate                         | 34.67                                    | 0.1039    | − 8.8 to 225.3   | 3.57(20), 3.14(25)                  |
| Diethyl 1,3-propanedioate<br>(malonate) | 33.91                                    | 0.1042    | − 49.9 to 199.3  | 2.15(20), 1.94(25)                  |
| Diethyl oxalate                         | 34.32                                    | 0.1119    | − 40.6 to 185.4  | 2.311(15), 1.618(30)                |
| Diethyl <i>o</i> -phthalate             | 38.47                                    | 0.0963    | − 40 to 295      | 9.18(35), 6.41(45)                  |
| Diethyl succinate                       | 33.97                                    | 0.1041    | − 21 to 217.7    |                                     |
| Diethyl sulfate                         | 35.47                                    | 0.0976    | − 25 to 208      |                                     |
| Diethyl sulfide                         | 27.33                                    | 0.1106    | − 104 to 92.1    | 0.558(0), 0.422(25)                 |
| 1,2-Dihydroxybenzene                    | 47.6                                     | 0.0849    | 104 to 245.5     |                                     |
| 1,3-Dihydroxybenzene                    | 54.8                                     | 0.0717    | 110 to 276       |                                     |
| Diiodomethane                           | 70.21                                    | 0.1613    | 6 to 181         |                                     |
| Diisobutylamine                         | 24.00                                    | 0.0912    | − 77 to 139      |                                     |
| Diisopentyl ether                       | 24.76                                    | 0.0871    | up to 172.5      | 1.40(11), 1.012(20)                 |
| Diisopropylamine                        | 21.03                                    | 0.1077    | − 61 to 83.5     | 0.393(25), 0.300(50), 0.237(75)     |
| Diisopropyl ether                       | 19.89                                    | 0.1048    | − 87 to 68       | 0.379(25)                           |
| 1,2-Dimethoxybenzene                    | 34.4                                     | 0.0642    | 22.5 to 206      | 3.281(25), 2.184(40)                |
| 1,1-Dimethoxyethane                     | 23.90                                    | 0.1159    | − 113 to 64.5    |                                     |
| 1,2-Dimethoxyethane                     | 48.0(25)                                 |           | − 68 to 85       | 0.670(− 10), 0.530(10), 0.455(25)   |
| Dimethoxymethane                        | 23.59                                    | 0.1199    | − 104.8 to 42    | 0.340(15), 0.325(20)                |
| <i>N,N</i> -Dimethylacetamide           | 32.40(30)                                | 29.50(50) | − 20 to 165.5    | 1.956(25), 1.279(50), 0.896(75)     |
| Dimethylamine                           | 29.50                                    | 0.1265    | − 92 to 6.9      | 0.300(− 25), 0.232(0)               |
| <i>N,N</i> -Dimethylaniline             | 38.14                                    | 0.1049    | 2.5 to 194       | 1.300(25), 0.911(50), 0.675(75)     |
| 2,4-Dimethylaniline                     | 39.34                                    | 0.0996    | − 14 to 214      |                                     |
| 2,2-Dimethylbutane                      | 18.29                                    | 0.0990    | − 100 to 49.7    | 0.351(25), 0.330(30)                |
| 2,3-Dimethylbutane                      | 19.38                                    | 0.1000    | − 128 to 58      | 0.361(25), 0.342(30)                |
| 2,3-Dimethyl-1-butanol                  | 26.22                                    | 0.0992    | − 14 to 118      |                                     |
| Dimethyl carbonate                      | 31.94                                    | 0.1343    | 0.5 to 91        |                                     |
| 1,1-Dimethylcyclopentane                | 23.78                                    | 0.1016    | − 70 to 87.5     |                                     |
| Dimethyl ether                          | 14.97                                    | 0.1478    | − 141 to − 24.9  |                                     |
| <i>N,N</i> -Dimethylformamide           | 36.76(20)                                | 34.40(40) | − 60 to 153      | 1.176(0), 0.794(25), 0.624(50)      |
| 2,4-Dimethylheptane                     | 23.21                                    | 0.0929    | < − 100 to 133   |                                     |
| 2,5-Dimethylheptane                     | 23.21                                    | 0.0929    | < − 100 to 136   |                                     |

**TABLE 5.16** Viscosity and Surface Tension of Various Organic Substances (*Continued*)

| Substance                          | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |           | Liquid range, °C | Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|------------------------------------|-----------------------------------------------------|-----------|------------------|-----------------------------------------------------------|
|                                    | <i>a</i>                                            | <i>b</i>  |                  |                                                           |
| 2,6-Dimethylheptane                | 22.17                                               | 0.0887    | − 103 to 135     |                                                           |
| Dimethyl hexanedioate              | 38.26                                               | 0.1138    | 8 to > 112       | 14(20)                                                    |
| Dimethyl maleate                   | 40.73                                               | 0.1220    | − 19 to 202      | 3.54(20), 3.21(25)                                        |
| Dimethyl malonate                  | 39.72                                               | 0.1208    | − 62 to 181      |                                                           |
| 2,2-Dimethylpentane                | 19.94                                               | 0.0957    | − 124 to 79      |                                                           |
| 2,3-Dimethylpentane                | 21.96                                               | 0.0995    | up to 90         | 0.406(20)                                                 |
| 2,4-Dimethylpentane                | 20.09                                               | 0.0972    | − 120 to 80.4    | 0.361(20)                                                 |
| 3,3-Dimethylpentane                | 21.59                                               | 0.0996    | − 135 to 86      |                                                           |
| 2,4-Dimethylphenol                 | 34.57                                               | 0.0869    | 24.5 to 211      |                                                           |
| 2,5-Dimethylphenol                 | 36.72                                               | 0.0850    | 74.5 to 211.5    | 1.55(80)                                                  |
| 3,4-Dimethylphenol                 | 35.75                                               | 0.0910    | 61 to 227        | 3.00(80)                                                  |
| 3,5-Dimethylphenol                 | 34.09                                               | 0.0807    | 64 to 222        | 2.42(80)                                                  |
| Dimethyl <i>o</i> -phthalate       |                                                     |           | 5.5 to 284       | 14.4(25), 5.309(50), 2.824(75)                            |
| 2,2-Dimethylpropane                | 12.05(20)                                           | 10.98(30) | − 16.6 to 9.5    | 0.328(0), 0.303(5)                                        |
| Dimethyl succinate                 | 39.00                                               | 0.1191    | 19 to 196.4      |                                                           |
| Dimethyl sulfate                   | 41.26                                               | 0.1163    | − 31.8 to 188    |                                                           |
| Dimethyl sulfide                   | 26.07                                               | 0.0805    | − 98 to 37       | 0.356(0), 0.289(20), 0.265(36)                            |
| Dimethyl sulfite                   | 36.48                                               | 0.1253    | up to 127        | 0.715(30), 0.436(80)                                      |
| Dimethyl sulfoxide                 | 43.54(20)                                           | 42.41(30) | 18.5 to 189      | 2.47(20), 1.192(55), 0.849(80)                            |
| 1,4-Dioxane                        | 36.23                                               | 0.1391    | 11.8 to 101.2    | 1.439(15), 1.087(30), 0.787(50)                           |
| Dipentyl ether                     | 26.66                                               | 0.0925    | − 69 to 190      | 1.188(15), 0.922(30)                                      |
| Dipentyl <i>o</i> -phthalate       | 32.56                                               | 0.0739    |                  | 17.03(35), 11.51(45)                                      |
| Dipentyl sulfide                   | 29.55                                               | 0.0876    |                  |                                                           |
| Dipentylamine                      | 45.36                                               | 0.1017    | 53 to 302        | 4.66 (55), 1.04(130)                                      |
| Diphenyl ether                     | 28.70                                               | 0.0780    | 27 to 258        | 2.130(50), 1.407(75), 1.023(100)                          |
| 1,2-Dipropoxyethane                | 25.03                                               | 0.0972    |                  |                                                           |
| Dipropoxymethane                   | 25.17                                               | 0.0953    |                  |                                                           |
| Dipropylamine                      | 24.86                                               | 0.1022    | − 63 to 109      | 0.517(25), 0.377(50), 0.288(75)                           |
| Dipropyl carbonate                 | 28.94                                               | 0.1015    | up to 168        |                                                           |
| Dipropylene glycol butyl ether     | 28.2(25)                                            |           | up to > 103      | 4.23(25)                                                  |
| Dipropylene glycol ethyl ether     | 27.7(25)                                            |           |                  | 3.11(25)                                                  |
| Dipropylene glycol isopropyl ether | 25.9(25)                                            |           | up to 80         | 386(25)                                                   |
| Dipropylene glycol methyl ether    | 28.8(25)                                            |           | − 117 to 188     | 3.1(25)                                                   |
| Dipropyl ether                     | 22.60                                               | 0.1047    | − 126 to 89.6    | 0.542(0), 0.396(25), 0.304(50)                            |
| Dodecane                           | 27.12                                               | 0.0884    | − 10 to 216      | 2.277(0), 1.378(25), 0.930(50)                            |
| 1-Dodecanol                        | 31.25                                               | 0.0748    | 24 to 259        |                                                           |
| Epichlorohydrin                    | 39.76                                               | 0.1360    | − 26 to 117      | 1.20(25)                                                  |
| 1,2-Epoxybutane                    | 23.9(20)                                            |           | − 150 to 63      | 0.419(15), 0.358(30)                                      |
| 1,2-Ethanediamine                  | 44.77                                               | 0.1398    | 11 to 117.3      | 1.54(20), 1.226(30)                                       |
| 1,2-Ethanediol                     | 50.21                                               | 0.0890    | − 12.6 to 197.3  | 26.09(15), 13.55(30)                                      |
| Ethanesulfonic acid                | 45.74                                               | 0.0824    | − 17 to > 123    |                                                           |
| Ethanesulfonyl chloride            | 43.43                                               | 0.1177    | up to 177        |                                                           |
| Ethanethiol                        | 25.06                                               | 0.0793    | − 148 to 35      | 0.364(0), 0.287(25)                                       |
| Ethanol                            | 24.05                                               | 0.0832    | − 114 to 78      | 1.786(0), 1.074(25), 0.694(50)                            |
| Ethanolamine                       | 51.11                                               | 0.1117    | 10.5 to 171      | 21.1(25), 8.560(50), 3.935(75)                            |
| Ethoxybenzene (phenetol)           | 35.17                                               | 0.1104    | − 29.5 to 170    | 1.364(15), 1.197(25), 0.817(50)                           |
| 2-Ethoxyethanol                    | 30.59                                               | 0.0897    | − 70 to 135      | 2.04(20), 1.85(25)                                        |
| Ethyl acetate                      | 26.29                                               | 0.1161    | − 84 to 77       | 0.578(0), 0.423(25), 0.325(50)                            |

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                     | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup> |
|-------------------------------|------------------------------------------|-----------|------------------|-------------------------------------|
|                               | <i>a</i>                                 | <i>b</i>  |                  |                                     |
| Ethyl acetoacetate            | 34.42                                    | 0.1015    | – 45 to 181      | 1.419(20), 1.508(25)                |
| Ethylamine                    | 22.63                                    | 0.1372    | – 81 to 16.6     |                                     |
| <i>N</i> -Ethylaniline        | 39.00                                    | 0.1070    | – 63.5 to 203    | 2.047(25), 1.231(50), 0.825(75)     |
| Ethylbenzene                  | 31.48                                    | 0.1094    | – 95 to 136      | 1360.631(25), 0.482(50), 0.380(75)  |
| Ethyl benzoate                | 37.16                                    | 0.1059    | – 35 to 212      | 2.407(15), 1.751(30)                |
| Ethyl butanoate               | 26.55                                    | 0.1045    | – 98 to 121      | 0.771(15), 0.613(25)                |
| 2-Ethylbutanoic acid          | 26.3(20)                                 |           | – 14 to 194      | 3.3(20)                             |
| 2-Ethyl-1-butanol             | 25.06(15)                                | 24.32(25) | < – 15 to 146    | 8.021(15), 5.892(25)                |
| Ethyl carbamate               |                                          |           | 50 to 184        | 0.916(105), 0.715(120)              |
| Ethyl chloroacetate           | 34.18                                    | 0.1177    | – 21 to 144      |                                     |
| Ethyl chloroformate           | 28.90                                    | 0.1084    | – 81 to 93       |                                     |
| Ethyl <i>trans</i> -cinnamate | 39.99                                    | 0.1045    | 10 to 271        | 8.7(20)                             |
| Ethyl crotonate               | 29.31                                    | 0.1066    | up to 138        |                                     |
| Ethyl cyanoacetate            | 38.80                                    | 0.1092    | – 22 to 206      | 3.256(15), 2.148(30)                |
| Ethylcyclohexane              | 27.78                                    | 0.1054    | – 111 to 132     | 1.139(0), 0.784(25), 0.579(50)      |
| Ethyl dichloroacetate         | 34.89                                    | 0.1158    | up to 155        |                                     |
| Ethyl dodecanoate             | 30.05                                    | 0.0863    | – 10 to 271      |                                     |
| Ethylene carbonate            |                                          |           | 36 to 248        | 1.85(40)                            |
| Ethylenediamine               | 44.77                                    | 0.1398    | 11 to 117        | 1.540(18)                           |
| Ethylene glycol               | 50.21                                    | 0.0890    | up to 198        | 26.09(15), 13.35(30), 6.554(50)     |
| Ethyleneimine                 | 7.9(20)                                  |           | – 78 to 56       | 0.418(25)                           |
| Ethylene oxide                | 27.66                                    | 0.1664    | – 111 to 10.6    | 0.3(0)                              |
| Ethyl formate                 | 26.47                                    | 0.1315    | – 80 to 54       | 0.419(15), 0.358(30), 0.300(50)     |
| Ethyl fumarate                | 33.90                                    | 0.1056    | 68 to > 148      |                                     |
| Ethylhexadecanoate            | 32.86                                    | 0.0859    | 22 to > 191      |                                     |
| Ethyl hexanoate               | 27.73                                    | 0.0960    | up to 168        |                                     |
| 2-Ethyl-1-hexanol             | 30.0(22)                                 |           | – 70 to 185      | 6.271(25), 2.631(50), 1.360(75)     |
| Ethyl isobutanoate            | 25.33                                    | 0.1046    | – 88 to 110      |                                     |
| Ethyl isothiocyanate          | 38.69                                    | 0.1326    | – 6 to 132       |                                     |
| Ethyl lactate                 | 30.72                                    | 0.0983    | – 26 to 155      | 2.44(25)                            |
| Ethyl 3-methylbutanoate       | 25.79                                    | 0.1006    | – 99 to 135      |                                     |
| Ethyl methyl ether            | 18.56                                    | 0.1317    | – 113 to 7.4     |                                     |
| Ethyl methyl sulfide          | 27.63                                    | 0.1286    | – 106 to 67      | 0.373(20), 0.354(25)                |
| Ethyl nitrate                 | 30.81                                    | 0.1345    | – 95 to 88       |                                     |
| 3-Ethylpentane                | 22.52                                    | 0.1032    | – 119 to 93.5    |                                     |
| Ethyl pentanoate              | 27.15                                    | 0.0999    | – 91 to 145      | 0.847(20)                           |
| Ethyl propanoate              | 26.72                                    | 0.1168    | – 74 to 99       | 0.564(15), 0.473(30), 0.380(50)     |
| Ethyl propyl ether            | 21.92                                    | 0.1054    | – 79 to 63       | 0.401(0), 0.323(20), 0.225(60)      |
| Ethyl salicylate              | 31.00                                    | 0.1091    | 2 to 234         | 1.772(45)                           |
| Ethyl thiocyanate             | 37.28                                    | 0.1226    | up to 145        |                                     |
| <i>o</i> -Ethyltoluene        | 32.33                                    | 0.1060    | – 81 to 165      |                                     |
| <i>p</i> -Ethyltoluene        | 30.98                                    | 0.1075    | – 62 to 162      |                                     |
| Ethyl trichloroacetate        | 32.97                                    | 0.1073    | up to 168        |                                     |
| Fluorobenzene                 | 29.67                                    | 0.1204    | – 42 to 85       | 0.620(15), 0.517(30), 0.423(50)     |
| 1-Fluorohexane                | 23.41                                    | 0.1001    | – 103 to 93      |                                     |
| 1-Fluoropentane               | 22.81                                    | 0.1315    | – 120 to 63      |                                     |
| <i>o</i> -Fluorotoluene       |                                          |           | – 62 to 115      | 0.680(20), 0.601(30)                |
| <i>m</i> -Fluorotoluene       | 32.31                                    | 0.1257    | – 87 to 115      | 0.608(20), 0.534(30)                |
| <i>p</i> -Fluorotoluene       | 30.44                                    | 0.1109    | – 56 to 117      | 0.622(20), 0.522(30)                |

**TABLE 5.16** Viscosity and Surface Tension of Various Organic Substances (*Continued*)

| Substance                      | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |           | Liquid range, °C | Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|--------------------------------|-----------------------------------------------------|-----------|------------------|-----------------------------------------------------------|
|                                | <i>a</i>                                            | <i>b</i>  |                  |                                                           |
| Formamide                      | 59.13                                               | 0.0842    | 2.6 to 220       | 4.320(15), 2.296(30), 1.833(50)                           |
| Formanilide                    | 44.30                                               | 0.0875    | 47 to 271        | 1.65(120)                                                 |
| Formic acid                    | 39.87                                               | 0.1098    | 8 to 101         | 1.966(15), 1.607(25), 1.030(50)                           |
| Furan                          | 24.10(20)                                           | 23.38(25) | −86 to 31        | 0.380(20), 0.361(25)                                      |
| 2-Furancarboxaldehyde          | 46.41                                               | 0.1327    | −36.5 to 162     | 2.501(0), 1.587(25), 1.143(50)                            |
| 2-Furanmethanol                | ca.<br>38(20)                                       |           | −31 to 171       | 4.62(25)                                                  |
| Glycerol                       | 63.14(17)                                           | 62.5(25)  | 18 to 290        | 934(25), 152(50), 39.8(75)                                |
| Glycerol tris(acetate)         | 37.88                                               | 0.081     |                  |                                                           |
| Glycerol tris(nitrate)         | 55.74                                               | 0.2504    | 13 to >160       | 36.0(20), 13.6(40)                                        |
| Glycerol tris(oleate)          | 36.03                                               | 0.0699    | −5 to >233       |                                                           |
| Glycerol tris(palmitate)       | 32.26                                               | 0.0672    | 65 to 320        |                                                           |
| Glycerol tris(sterate)         | 32.73                                               | 0.0685    |                  |                                                           |
| Heptanal                       | 28.64                                               | 0.0920    | −43 to 153       | 0.977(15)                                                 |
| Heptane                        | 22.10                                               | 0.0980    | −91 to 98        | 0.523(0), 0.416(20), 0.341(40)                            |
| Heptanoic acid                 | 29.88                                               | 0.0848    | −8 to 222        | 3.84(25), 2.282(50), 1.488(75)                            |
| 1-Heptanol                     |                                                     |           | −34 to 176       | 8.53(15), 5.810(25), 2.603(50)                            |
| 2-Heptanol                     |                                                     |           | up to 159        | 3.955(25), 1.799(50), 0.987(75)                           |
| 3-Heptanol                     |                                                     |           | −70 to 157       | 1.957(50), 0.976(75), 0.584(100)                          |
| 4-Heptanol                     |                                                     |           |                  | 4.207(25), 1.695(50), 0.882(75)                           |
| 2-Heptanone                    | 28.76                                               | 0.1056    | −35 to 151       | 0.854(15), 0.686(30), 0.407(50)                           |
| 4-Heptanone                    | 28.11                                               | 0.1060    | −32 to 143.7     | 0.736(20)                                                 |
| 1-Heptene                      | 22.28                                               | 0.0991    | −120 to 93.6     | 0.441(0), 0.340(25), 0.273(50)                            |
| Heptylamine                    | 25.96                                               | 0.0783    | −23 to 156       | 1.314(25), 0.865(50), 0.600(75)                           |
| Hexadecane                     | 29.18                                               | 0.0854    | 18.2 to 286.8    | 3.032(25), 1.879(50), 1.260(75)                           |
| 1,5-Hexadiene                  | 20.93                                               | 0.1028    | −140.7 to 59.5   | 0.275(20), 0.244(36)                                      |
| Hexafluorobenzene              | 22.6(20)                                            |           | 5.1 to 80.3      | 2.789(25), 1.730(50), 1.151(75)                           |
| Hexamethyldisiloxane           | 17.01                                               | 0.0763    | −67 to 101       |                                                           |
| Hexamethylphosphoramide        | 33.8(20)                                            |           | 7 to 232         | 3.47(20)                                                  |
| Hexane                         | 20.44                                               | 0.1022    | −95.4 to 68.7    | 0.405(0), 0.313(20), 0.271(40)                            |
| Hexanenitrile                  | 29.64                                               | 0.0907    | −80 to 163.6     | 1.041(15), 0.830(30), 0.650(50)                           |
| Hexanoic acid                  | 28.05(20)                                           | 27.55(25) | −3 to 205        | 3.525(15), 2.511(30)                                      |
| 1-Hexanol                      | 27.81                                               | 0.0801    | −44.6 to 157.5   | 6.203(15), 3.872(30), 2.271(50)                           |
| 2-Hexanone                     | 28.18                                               | 0.1092    | −55.5 to 127.6   | 0.584(25), 0.429(50), 0.329(75)                           |
| 1-Hexene                       | 20.47                                               | 0.1027    | −140 to 63.5     | 0.326(0), 0.252(25), 0.202(50)                            |
| Hexyl acetate                  | 28.44                                               | 0.0970    | −81 to 171       |                                                           |
| 4-Hydroxy-4-methyl-2-pentanone | 31.0(20)                                            |           | −44 to 168       | 6.621(0), 2.798(25), 1.829(50)                            |
| Iodobenzene                    | 41.52                                               | 0.1123    | −31 to 188       | 1.554(25), 1.117(50), 0.854(75)                           |
| 1-Iodobutane                   | 30.82                                               | 0.1031    | −103.5 to 131    |                                                           |
| 2-Iodobutane                   | 30.32                                               | 0.1056    | −104 to 120      |                                                           |
| Iodoethane                     | 31.67                                               | 0.1286    | −111 to 72.4     | 0.617(15), 0.540(30), 0.444(50)                           |
| 1-Iodoheptane                  | 32.18                                               | 0.0887    | −48 to 204       |                                                           |
| 1-Iodohexadecane               | 34.49                                               | 0.0880    | 23 to >207       |                                                           |
| 1-Iodohexane                   | 31.63                                               | 0.0845    | up to 180        |                                                           |
| Iodomethane                    | 33.42                                               | 0.1234    | −66.5 to 42.5    | 0.594(0), 0.500(20), 0.424(40)                            |
| 1-Iodo-2-methylpropane         | 30.26                                               | 0.1072    | −93.5 to 121     | 0.875(20), 0.697(40)                                      |
| 1-Iodoctane                    | 32.51                                               | 0.0915    | −46 to 226       |                                                           |
| 1-Iodopentane                  | 31.41                                               | 0.1014    | −85 to 155       |                                                           |
| 1-Iodopropane                  | 31.64                                               | 0.1136    | −101 to 102.6    | 0.837(15), 0.670(30), 0.541(50)                           |

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                     | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup> |
|-------------------------------|------------------------------------------|-----------|------------------|-------------------------------------|
|                               | <i>a</i>                                 | <i>b</i>  |                  |                                     |
| 2-Iodopropane                 | 29.35                                    | 0.1107    | − 90 to 89.5     | 0.732(15), 0.620(30), 0.506(50)     |
| <i>p</i> -Iodotoluene         | 39.23                                    | 0.0965    | up to 211        |                                     |
| α-Ionone                      | 34.10                                    | 0.0949    | > 124            |                                     |
| β-Ionone                      | 35.36                                    | 0.0950    | > 128            |                                     |
| Isobutanenitrile              | 24.93(20)                                | 23.84(30) | − 71.5 to 104    | 0.551(15), 0.456(30)                |
| Isobutyl acetate              | 25.59                                    | 0.1013    | − 99 to 116.5    | 0.676(25), 0.493(50), 0.370(75)     |
| Isobutylamine                 | 24.48                                    | 0.1092    | − 86.6 to 68     | 0.770(0), 0.571(25), 0.367(50)      |
| Isobutylbenzene               | 29.39                                    | 0.0961    | − 51.5 to 172.8  |                                     |
| Isobutyl formate              | 26.14                                    | 0.1122    | − 95.5 to 98.4   | 0.680(20)                           |
| Isobutyl propanoate           | 30.92                                    | 0.1270    | − 71 to 137      |                                     |
| Isopentyl acetate             | 26.75                                    | 0.0989    | − 78.5 to 142    | 0.872(20), 0.790(25)                |
| Isophorone                    |                                          |           | − 8.1 to 215.2   | 4.201(0), 2.329(25), 1.415(50)      |
| Isopropyl acetate             | 24.44                                    | 0.1072    | − 73 to 89       | 0.559(20)                           |
| Isopropylamine                | 19.91                                    | 0.0972    | − 95 to 31.7     | 0.454(0), 0.325(25)                 |
| Isopropylbenzene              | 30.32                                    | 0.1054    | − 96 to 154      | 1.075(0), 0.737(25), 0.547(50)      |
| Isopropyl formate             | 24.56                                    | 0.1147    |                  | 0.512(20)                           |
| Lactonitrile                  | 38.31                                    | 0.0960    | − 40 to > 103    | 2.01(30)                            |
| D-Limonene                    | 29.50                                    | 0.0929    | − 96.5 to 178    |                                     |
| (±)-Mandelonitrile            | 45.90                                    | 0.0988    | − 10 to 170      |                                     |
| Methacrylic acid              | 26.5(25)                                 |           | 16 to 163        | 1.32(20)                            |
| Methacrylonitrile             | 24.4(20)                                 |           | − 35.8 to 90.3   | 0.392(20)                           |
| Methanesulfonic acid          | 52.28                                    | 0.0893    | 20 to > 167      |                                     |
| Methanethiol                  | 28.09                                    | 0.1696    | − 123 to 6.0     |                                     |
| Methanol                      | 24.00                                    | 0.0773    | − 97.7 to 64.7   | 0.793(0), 0.676(10), 0.544(25)      |
| <i>o</i> -Methoxybenzaldehyde | 45.34                                    | 0.1105    | 37 to 238        |                                     |
| <i>p</i> -Methoxybenzaldehyde | 44.69                                    | 0.1047    | − 1 to 248       |                                     |
| Methoxybenzene                | 38.11                                    | 0.1204    | − 37.5 to 153.8  | 1.152(15), 1.056(25), 0.747(50)     |
| 2-Methoxyethanol              | 33.30                                    | 0.0984    | − 85.1 to 124    | 1.71(20), 1.60(25)                  |
| 2-(2-Methoxyethoxy)ethanol    | 34.8(25)                                 | 29.9(75)  | − 50 to 194      | 3.48(25), 1.61(60)                  |
| 1-Methoxy-2-nitrobenzene      | 48.62                                    | 0.1185    | 10.5 to 277      |                                     |
| <i>o</i> -Methoxyphenol       | 41.2                                     | 0.0943    | 28 to 205        |                                     |
| <i>p</i> -Methoxytoluene      | 36.20                                    | 0.1071    | up to 174        |                                     |
| <i>N</i> -Methylacetamide     | 33.67(30)                                | 30.62(50) | 30.6 to 206      | 3.88(30), 2.54(45)                  |
| Methyl acetate                | 27.95                                    | 0.1289    | − 98 to 57       | 0.477(0), 0.364(25), 0.284(50)      |
| Methyl acetoacetate           | 34.98                                    | 0.0944    | 27.5 to 171.7    |                                     |
| Methyl acrylate               |                                          |           | − 76.5 to 80.2   | 1.398(20)                           |
| Methylamine                   | 22.87                                    | 0.1488    | − 93.5 to − 6.3  | 0.319(− 25)                         |
| <i>N</i> -Methylaniline       | 39.32                                    | 0.0970    | − 57 to 196      | 2.042(25), 1.222(50), 0.825(75)     |
| <i>o</i> -Methylaniline       |                                          |           |                  | 3.823(25), 1.936(50), 1.198(75)     |
| <i>m</i> -Methylaniline       |                                          |           |                  | 3.306(25), 1.679(50), 1.014(75)     |
| Methyl benzoate               | 40.10                                    | 0.1171    | − 15 to 199.5    | 2.298(15), 0.206(20), 1.673(30)     |
| 2-Methyl-1,2-butadiene        |                                          |           |                  | 0.266(0.3), 0.233(20)               |
| 2-Methylbutane                | 17.20                                    | 0.1103    | up to 30         | 0.376(− 25), 0.277(0), 0.214(25)    |
| Methyl butanoate              | 27.48                                    | 0.1145    | − 85.8 to 103    | 0.580(20), 0.459(40), 0.406(50)     |
| 3-Methylbutanoic acid         | 27.28                                    | 0.0886    | − 29.3 to 176.5  | 2.731(15), 2.411(20)                |
| 2-Methyl-1-butanol            | 21.5(25)                                 |           | < − 70 to 128    | 5.50(20), 4.453(25), 1.963(50)      |
| 2-Methyl-2-butanol            | 24.18                                    | 0.0748    | − 9.0 to 102.0   | 5.48(15), 2.81(30)                  |
| 3-Methyl-1-butanol            | 25.76                                    | 0.0820    | − 117 to 131     | 4.81(15), 2.96(30), 1.842(50)       |
| 3-Methyl-2-butanol            | 23.0(25)                                 |           | up to 112.9      | 3.51(25)                            |

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                                          | Surface tension,<br>mN · m <sup>-1</sup> |                           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup>                                              |
|----------------------------------------------------|------------------------------------------|---------------------------|------------------|----------------------------------------------------------------------------------|
|                                                    | <i>a</i>                                 | <i>b</i>                  |                  |                                                                                  |
| 2-Methyl-1-butene                                  | 18.81                                    | 0.1148                    | − 137.6 to 31    | 0.872(20)                                                                        |
| 2-Methyl-2-butene                                  | 19.70                                    | 0.1271                    | − 133.8 to 38.6  |                                                                                  |
| 3-Methyl-1-butene                                  | 16.42                                    | 0.1031                    | − 168 to 20      |                                                                                  |
| 2-Methylbutyl acetate                              | 26.75                                    | 0.0989                    | − 99 to 117      |                                                                                  |
| 3-Methylbutyronitrile                              | 27.58                                    | 0.0827                    | − 101 to 129     |                                                                                  |
| Methyl chloroacetate                               | 37.90                                    | 0.1304                    | − 32 to 130      |                                                                                  |
| Methyl cyanoacetate                                | 41.32                                    | 0.1074                    | − 22.5 to 201    |                                                                                  |
| Methylcyclohexane                                  | 26.11                                    | 0.1130                    | − 126.6 to 100.9 |                                                                                  |
| <i>cis</i> -2-Methylcyclohexanol                   | 32.45                                    | 0.0770<br>(mixed isomers) | 7 to 165         | 18.08(25), 13.60(30)                                                             |
| <i>trans</i> -2-Methylcyclohexanol                 |                                          |                           | − 2 to 167.5     | 37.13(25), 25.14(30)                                                             |
| <i>cis</i> -3-Methylcyclohexanol                   | 29.08                                    | 0.0629<br>(mixed isomers) | − 6 to 168       | 19.7(25), 17.23(30)                                                              |
| <i>trans</i> -3-Methylcyclohexanol                 | 28.80(30)                                |                           | − 0.5 to 167     | 25.62(16), 15.60(30)                                                             |
| <i>cis</i> -4-Methylcyclohexanol                   | 29.07                                    | 0.0690<br>(mixed isomers) | − 9.2 to 173     |                                                                                  |
| 2-Methylcyclohexanone                              | 34.06                                    | 0.1027                    | up to 162        |                                                                                  |
| 3-Methylcyclohexanone                              | 33.06                                    | 0.0925                    | up to 169        |                                                                                  |
| 4-Methylcyclohexanone                              | 32.83                                    | 0.0935                    | up to 171        |                                                                                  |
| Methylcyclopentane                                 | 24.63                                    | 0.1163                    | − 142.2 to 71.8  |                                                                                  |
| Methyl decanoate                                   | 30.33                                    | 0.0912                    | − 18 to 223      |                                                                                  |
| Methyl dichloroacetate                             | 37.00                                    | 0.1219                    | − 52 to 143      |                                                                                  |
| Methyl dodecanoate                                 | 31.37                                    | 0.0893                    | 4.8 to 262       | 1.678(25), 1.155(50), 0.824(75)<br>0.424(0), 0.360(15), 0.325(25)                |
| <i>N</i> -Methylformamide                          | 37.96(30)                                | 35.02(50)                 | − 4 to 199.5     |                                                                                  |
| Methyl formate                                     | 28.29                                    | 0.1572                    | − 99 to 31.7     |                                                                                  |
| Methyl heptanoate                                  | 28.95                                    | 0.0987                    | − 55.8 to 173.5  |                                                                                  |
| 4-Methyl-3-heptanol                                |                                          |                           | − 123 to 170     |                                                                                  |
| 5-Methyl-3-heptanol                                |                                          |                           | − 91 to 172      |                                                                                  |
| Methyl hexadecanoate<br>(palmitate)                | 31.50                                    | 0.0775                    | 32 to > 196      |                                                                                  |
| 2-Methylhexane                                     | 21.22                                    | 0.0966                    | − 118 to 90      |                                                                                  |
| 3-Methylhexane                                     | 21.73                                    | 0.0970                    | − 119 to 92      | 0.378(20)<br>0.372(20), 0.350(25)<br>0.672(0), 0.523(20), 0.419(40)<br>3.402(20) |
| Methyl hexanoate                                   | 28.47                                    | 0.1045                    | − 71 to 151      |                                                                                  |
| Methyl isobutanoate                                | 25.99                                    | 0.1131                    | − 84.7 to 92.5   |                                                                                  |
| 1-Methyl-4-isopropylbenzene<br>( <i>p</i> -cymene) | 28.83                                    | 0.0877                    |                  |                                                                                  |
| Methyl methacrylate                                | 28-<br>29(30)                            |                           | − 48 to 100      |                                                                                  |
| 1-Methylnaphthalene                                | 39.96                                    | 0.0934                    | − 30.4 to 245    |                                                                                  |
| Methyl octadecanoate                               | 32.20                                    | 0.0775                    | 38 to > 215      |                                                                                  |
| 2-Methyloctane                                     | 23.76                                    | 0.0940                    | − 80.3 to 143.2  |                                                                                  |
| 4-Methyloctane                                     | 24.22                                    | 0.0940                    | − 113 to 142     | 4.88(20)<br>0.372(0), 0.286(25), 0.226(50)<br>0.395(0), 0.307(25), 0.292(30)     |
| Methyl octanoate                                   | 29.93                                    | 0.1002                    | − 40 to 192.9    |                                                                                  |
| Methyl oleate                                      | 31.3(25)                                 | 25.4(100)                 | − 19.9 to > 218  |                                                                                  |
| 2-Methylpentane                                    | 19.37                                    | 0.0997                    | − 154 to 60.3    |                                                                                  |
| 3-Methylpentane                                    | 20.26                                    | 0.1060                    | − 163 to 63      |                                                                                  |



TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                        | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup> |
|----------------------------------|------------------------------------------|-----------|------------------|-------------------------------------|
|                                  | <i>a</i>                                 | <i>b</i>  |                  |                                     |
| 4-Methylpentanenitrile           | 28.89                                    | 0.0917    | − 51.1 to 156.5  | 0.980(20), 0.843(30)                |
| Methyl pentanoate                | 27.85                                    | 0.1044    | up to 128        | 0.713(20)                           |
| 2-Methyl-1-pentanol              | 26.98                                    | 0.0819    | up to 148        |                                     |
| 3-Methyl-1-pentanol              | 26.92                                    | 0.0789    | up to 153        |                                     |
| 4-Methyl-1-pentanol              | 25.93                                    | 0.0743    | up to 152        |                                     |
| 2-Methyl-2-pentanol              | 25.07                                    | 0.0861    | − 103 to 121     |                                     |
| 3-Methyl-2-pentanol              | 27.14                                    | 0.0919    | up to 134        |                                     |
| 4-Methyl-2-pentanol              | 24.67                                    | 0.0821    | − 90 to 122      | 4.074(25)                           |
| 2-Methyl-3-pentanol              | 26.43                                    | 0.0914    | up to 126        |                                     |
| 3-Methyl-3-pentanol              | 25.48                                    | 0.0888    | − 23.6 to 123    |                                     |
| 4-Methyl-2-pentanone             | 23.64(20)                                | 19.62(60) | − 84 to 116.5    | 0.585(20), 0.522(30), 0.406(50)     |
| Methyl phenyl sulfide            | 42.81                                    | 0.1238    | − 15 to 188      |                                     |
| <i>N</i> -Methyl propanamide     | 31.29(20)                                | 29.12(50) | − 43 to > 146    | 6.06(20), 4.58(30), 3.56(40)        |
| 2-Methylpropanenitrile           |                                          |           | − 72 to 108      | 0.551(15), 0.456(30)                |
| Methyl propanoate                | 27.58                                    | 0.1258    | − 88 to 80       | 0.581(0), 0.431(25), 0.333(50)      |
| 2-Methylpropanoic acid           | 25.55(20)                                | 25.13(25) | − 47 to 154      | 1.857(0), 1.226(25), 0.863(50)      |
| 2-Methyl-1-propanol              | 24.53                                    | 0.0795    | − 108 to 108     | 4.70(15), 2.876(30)                 |
| 2-Methyl-2-propanol              | 20.02(15)                                | 19.10(30) | 25.8 to 82.4     | 1.421(50), 0.678(75)                |
| 2-Methylpropene                  | 14.84                                    | 0.1319    | − 140 to − 6.9   |                                     |
| 1-Methylpropyl acetate           | 25.72                                    | 0.1054    |                  |                                     |
| 2-Methyl-1-propylamine           | 24.48                                    | 0.1092    | − 87 to 68       | 21.7(25)                            |
| 2-Methylpropyl formate           | 26.14                                    | 0.1122    | − 96 to 98       | 0.680(20)                           |
| 2-Methylpyridine                 | 36.11                                    | 0.1243    | − 66.7 to 129    | 0.805(20), 0.710(30)                |
| 3-Methylpyridine                 | 37.35                                    | 0.1153    | − 18.3 to 144    |                                     |
| 4-Methylpyridine                 | 37.71                                    | 0.1141    | 3.8 to 145       |                                     |
| <i>N</i> -Methyl-2-pyrrolidinone |                                          |           | − 24.4 to 202    | 1.666(25)                           |
| Methyl salicylate                | 42.15                                    | 0.1174    | − 8 to 223       | 1.102(75), 0.815(100)               |
| Methyl tetradecanoate            | 31.00                                    | 0.0800    | 18.4 to 323      |                                     |
| 2-Methyltetrahydrofuran          |                                          |           | < − 75 to 78     | 0.777(− 20), 0.601(0), 0.536(10)    |
| Methyl thiocyanate               | 40.66                                    | 0.1305    | − 5 to 133       | 64.3(0)                             |
| Morpholine                       | 37.63(20)                                | 36.24(30) | − 4.9 to 128     | 2.53(15), 1.79(30), 1.247(50)       |
| Naphthalene                      |                                          |           | 80 to 217.7      | 0.967(80), 0.780(100)               |
| <i>p</i> -Nitroaniline           | 60.62                                    | 0.0923    | 147 to 332       |                                     |
| Nitrobenzene                     | 48.62                                    | 0.1185    | 5.8 to 210.8     | 2.165(15), 1.863(25), 1.262(50)     |
| Nitroethane                      | 35.27                                    | 0.1255    | − 90 to 114      | 0.940(0), 0.688(25), 0.526(50)      |
| Nitromethane                     | 40.72                                    | 0.1678    | − 28.4 to 101.2  | 0.692(15), 0.596(30), 0.481(50)     |
| 1-Nitro-2-methoxybenzene         | 48.62                                    | 0.1185    | 95 to 273        |                                     |
| <i>o</i> -Nitrophenol            | 47.35                                    | 0.1174    | 45 to 216        | 2.343(45)                           |
| 1-Nitropropane                   | 32.62                                    | 0.1009    | − 108 to 131.1   | 0.798(25), 0.589(50), 0.460(75)     |
| 2-Nitropropane                   | 32.18                                    | 0.1158    | − 91.3 to 120.3  | 0.750(25)                           |
| <i>o</i> -Nitrotoluene           | 44.10                                    | 0.1174    | − 10 to 222      | 2.37(20), 1.63(40)                  |
| <i>m</i> -Nitrotoluene           | 43.54                                    | 0.1118    | 15.5 to 231.9    | 0.233(20), 1.60(40)                 |
| <i>p</i> -Nitrotoluene           | 42.26                                    | 0.0974    | 52 to 238        | 1.20(60)                            |
| Nonane                           | 24.72                                    | 0.0935    | − 53.5 to 150.8  | 0.964(0), 0.666(25), 0.488(50)      |
| Nonanoic acid                    |                                          |           | 12.5 to 254.5    | 7.011(25), 3.712(50), 2.234(75)     |
| 1-Nonanol                        | 29.79                                    | 0.0789    | − 5.5 to 215     | 14.3(20), 9.123(25), 4.032(50)      |
| 5-Nonanone                       | 28.72                                    | 0.0975    | − 50 to 187      | 1.199(25), 0.834(50), 0.619(75)     |
| 1-Nonene                         | 24.90                                    | 0.0938    | − 81 to 146      | 0.620(20), 0.586(25)                |
| Octadecane                       | 29.98                                    | 0.0843    | 28.1 to 316.3    | 2.487(50), 1.609(75), 1.132(100)    |

**TABLE 5.16** Viscosity and Surface Tension of Various Organic Substances (*Continued*)

| Substance                              | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |           | Liquid range, °C | Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|----------------------------------------|-----------------------------------------------------|-----------|------------------|-----------------------------------------------------------|
|                                        | <i>a</i>                                            | <i>b</i>  |                  |                                                           |
| Octamethylcyclotetrasiloxane           | 20.19                                               | 0.0811    | 17 to 176        | 2.20(20)                                                  |
| Octane                                 | 23.52                                               | 0.0951    | − 56.8 to 125.7  | 0.546(20), 0.433(40), 0.355(60)                           |
| Octanenitrile                          | 29.61                                               | 0.0802    | − 45.6 to 205    | 1.811(15), 1.356(30)                                      |
| Octanoic acid                          | 29.21(20)                                           | 28.7(25)  | 16.6 to 239      | 5.020(25), 2.656(50), 1.654(75)                           |
| 1-Octanol                              | 29.09                                               | 0.0795    | − 15.5 to 195    | 10.64(15), 6.125(30), 3.232(50)                           |
| 2-Octanol                              | 27.96                                               | 0.0820    | − 31.6 to 180    |                                                           |
| 1-Octene                               | 23.68                                               | 0.0958    | − 102 to 121     | 0.470(20), 0.447(25)                                      |
| Oleic acid                             | 32.80(20)                                           | 27.94(90) | 13.4 to 360      | 38.80(20), 27.64(25)                                      |
| 4-Oxopentanoic acid                    | 41.69                                               | 0.0763    | 33 to 246        |                                                           |
| Paraldehyde                            | 28.28                                               | 0.1062    | 12.6 to 124      | 1.079(25), 0.692(50), 0.485(75)                           |
| Parathion                              | 39.2(25)                                            |           | 6 to 375         | 15.30(25)                                                 |
| Pentachloroethane                      | 37.09                                               | 0.1178    | − 29.9 to 160    | 2.741(15), 2.070(30), 1.491(50)                           |
| Pentadecane                            | 28.78                                               | 0.0857    | 9.9 to 270       | 2.814(22)                                                 |
| Pentanal                               | 27.96                                               | 0.1010    | − 92 to 103      |                                                           |
| Pentane                                | 18.25                                               | 0.1121    | − 129.7 to 36.0  | 0.351(− 25), 0.274(0), 0.224(25)                          |
| 1,5-Pentanediol                        | 43.2(20)                                            |           | − 18 to 239      | 128(20)                                                   |
| 2,4-Pentanedione                       | 33.28                                               | 0.1144    | − 23.1 to 138    | 0.6(20)                                                   |
| Pentanenitrile                         | 27.44(20)                                           | 26.33(30) | − 92 to 141.3    | 0.779(15), 0.637(30)                                      |
| Pentanoic acid                         | 28.90                                               | 0.0887    | − 33.7 to 186    | 2.359(15), 1.774(30), 0.979(70)                           |
| 1-Pentanol                             | 27.54                                               | 0.0874    | − 79 to 137.5    | 4.650(15), 3.619(25), 1.820(50)                           |
| 2-Pentanol                             | 25.96                                               | 0.1004    | − 73 to 119.3    | 5.130(15), 2.780(30), 1.447(50)                           |
| 3-Pentanol                             | 24.60(20)                                           | 23.76(30) | − 69 to 116      | 7.337(15), 3.306(30), 1.473(50)                           |
| 2-Pentanone                            | 24.89                                               | 0.0655    | − 76.8 to 102    | 0.641(0), 0.473(25), 0.362(50)                            |
| 3-Pentanone                            | 27.36                                               | 0.1047    | − 39.0 to 102    | 0.592(0), 0.444(25), 0.345(50)                            |
| 1-Pentene                              | 18.20                                               | 0.1099    | − 165 to 30.1    | 0.313(− 25), 0.241(0), 0.195(25)                          |
| <i>cis</i> -2-Pentene                  | 19.71                                               | 0.1172    | − 151 to 37.0    |                                                           |
| <i>trans</i> -2-Pentene                | 18.90                                               | 0.0997    | − 140 to 36.3    |                                                           |
| Pentyl acetate                         | 27.66                                               | 0.0994    | − 70.8 to 149.2  | 0.924(20), 0.862(25)                                      |
| Pentylamine                            | 24.4(13)                                            |           | − 55 to 104      | 1.030(0), 0.702(25), 0.493(50)                            |
| Phenol                                 | 43.54                                               | 0.1069    | 41 to 182        | 3.437(50), 1.784(75), 1.099(100)                          |
| 2-Phenylacetamide                      | 46.26                                               | 0.0788    | 157 to bp        |                                                           |
| Phenyl acetate                         |                                                     |           | < 45 to 196      | 1.799(45)                                                 |
| Phenylacetonitrile                     | 44.57                                               | 0.1155    | − 23.8 to 233.5  | 1.93(25)                                                  |
| 1-Phenylethanol                        | 42.88                                               | 0.1038    | 20 to 204        |                                                           |
| Phenylhydrazine                        | 48.14                                               | 0.1292    | 19.5 to 243      | 13.0(25), 4.553(50), 1.850(75)                            |
| Phenyl isothiocyanate                  | 42.73                                               | 0.1086    | − 30 to 163      |                                                           |
| Phenyl salicylate                      | 45.20                                               | 0.0976    | 44 to > 173      |                                                           |
| (±)- $\alpha$ -Pinene                  | 28.35                                               | 0.0944    | − 64 to 156      | 1.61(25)                                                  |
| <i>L</i> - $\beta$ -Pinene             | 28.26                                               | 0.0934    | − 61 to 166      | 1.70(20), 1.41(25)                                        |
| Piperidine                             | 31.79                                               | 0.1153    | − 11 to 106      | 1.573(25), 0.958(50), 0.649(75)                           |
| 1,2-Propanediol (see propylene glycol) |                                                     |           |                  |                                                           |
| 1,3-Propanediol                        | 47.43                                               | 0.0903    | − 27 to 214      | 56.0(20), 18.0(40)                                        |
| Propanenitrile (propionitrile)         | 29.63                                               | 0.1153    | − 92.8 to 97.2   | 0.294(25), 0.240(50), 0.202(75)                           |
| 1-Propanethiol                         | 27.38                                               | 0.1272    | − 113 to 68      | 0.503(0), 0.385(25)                                       |
| 2-Propanethiol                         | 24.26                                               | 0.1174    | − 131 to 52.6    | 0.477(0), 0.357(25), 0.280(50)                            |
| Propanoic acid                         | 28.68                                               | 0.0993    | − 20.5 to 141.1  | 1.030(25), 0.749(50), 0.569(75)                           |
| Propanoic anhydride                    | 30.30(20)                                           | 29.70(25) | − 45 to 170      | 1.144(20), 1.061(25)                                      |
| 1-Propanol                             | 25.26                                               | 0.0777    | − 127 to 97.2    | 2.522(15), 1.722(30), 1.107(50)                           |

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                         | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C  | Viscosity, mN · s · m <sup>-2</sup> |
|-----------------------------------|------------------------------------------|-----------|-------------------|-------------------------------------|
|                                   | <i>a</i>                                 | <i>b</i>  |                   |                                     |
| 2-Propanol                        | 22.90                                    | 0.0789    | − 89.5 to 82.4    | 2.859(15), 1.765(30), 1.028(50)     |
| 2-Propen-1-ol (allyl alcohol)     | 27.53                                    | 0.0902    | − 129 to 98       | 1.363(20), 0.914(40)                |
| Propionaldehyde (propanal)        |                                          |           | − 81 to 48        | 0.357(15), 0.321(25)                |
| Propionamide                      | 39.05                                    | 0.0909    | 79 to 222.2       |                                     |
| Propyl acetate                    | 26.60                                    | 0.1120    | − 93 to 101.6     | 0.768(0), 0.544(25), 0.406(50)      |
| Propylamine                       | 24.86                                    | 0.1243    | − 83 to 42.2      | 0.376(25)                           |
| Propylbenzene                     | 31.13                                    | 0.1075    | − 99.2 to 159.2   |                                     |
| Propyl benzoate                   | 36.55                                    | 0.1069    | − 51.6 to 98      |                                     |
| Propyl butanoate                  | 27.06                                    | 0.1000    | − 95 to 143       | 0.831(20)                           |
| 1,2-Propylene glycol              |                                          |           | − 60 to 188       | 40.4(0), 11.3(25), 4.770(50)        |
| Propyleneimine                    |                                          |           | up to 66          | 0.491(25)                           |
| 1,2-Propylene oxide               |                                          |           | − 112 to 34       | 0.327(20), 0.28(25)                 |
| Propyl formate                    | 26.77                                    | 0.1119    | − 92.9 to 80.9    | 0.669(0), 0.574(20), 0.417(40)      |
| Propyl isobutanoate               | 25.83                                    | 0.1015    | up to 135         | 0.831(20)                           |
| Propyl nitrate                    | 29.67                                    | 0.1237    | − 100 to 110.1    |                                     |
| Propyl pentanoate                 | 27.72                                    | 0.0984    | − 75.9 to 122.5   | 1.053(20)                           |
| Propyl propanoate                 | 26.85                                    | 0.1059    | − 76 to 122.5     | 0.673(20)                           |
| Propyne                           | 14.51                                    | 0.1482    | − 102.8 to − 23.2 |                                     |
| 2-Propyn-1-ol                     | 38.59                                    | 0.1270    | − 51.8 to 114     | 1.68(20)                            |
| Pyridazine                        | 50.55                                    | 0.1036    | − 8 to 208        |                                     |
| Pyridine                          | 39.82                                    | 0.1306    | − 41.6 to 115.2   | 1.361(0), 0.879(25), 0.637(50)      |
| Pyrimidine                        | 32.85                                    | 0.1010    | 22 to 124         |                                     |
| Pyrrole                           | 39.81                                    | 0.1100    | − 23.4 to 130     | 2.085(0), 1.225(25), 0.828(50)      |
| Pyrrolidine                       | 31.48                                    | 0.0900    | − 58 to 86.5      | 1.071(0), 0.704(25), 0.512(50)      |
| 2-Pyrrolidone                     |                                          |           | 25 to 251         | 13.3(25)                            |
| Quinoline                         | 45.25                                    | 0.1063    | − 15 to 237       | 3.337(25), 1.892(50), 1.201(75)     |
| Salicylaldehyde                   | 45.38                                    | 0.1242    | − 7 to 197        | 2.90(20), 1.71(30), 1.669(45)       |
| Squalane                          |                                          |           | − 38 to 350       | 6.08(20)                            |
| Squalene                          |                                          |           | − 75 to > 285     | 12(25)                              |
| Stearic acid                      |                                          |           | 67 to > 184       | 11.6(70)                            |
| Styrene                           | 32.0(20)                                 | 30.98(30) | − 31 to 145       | 1.050(0), 0.696(25), 0.507(50)      |
| Succinonitrile                    | 53.26                                    | 0.1079    | 54.5 to 266       | 2.591(60), 2.008(75)                |
| 1,1,2,2-Tetrabromoethane          | 52.37                                    | 0.1463    | 0 to 243.5        | 13.50(11), 9.797(20)                |
| 1,1,2,2-Tetrachlorodifluoroethane | 26.13                                    | 0.1133    | 26.0 to 92.8      | 1.21(25), 1.208(30)                 |
| 1,1,2,2-Tetrachloroethane         | 38.75                                    | 0.1268    | − 70.2 to 130.5   | 1.844(15), 1.456(30)                |
| Tetrachloroethylene               | 32.86(15)                                | 31.27(30) | − 22 to 121       | 1.932(15), 0.798(30), 0.654(53)     |
| Tetradecane                       | 28.30                                    | 0.0869    | 5.5 to 253.6      | 2.128(25), 1.376(50), 0.953(75)     |
| Tetradecanoic acid                | 33.90                                    | 0.0932    | 54 to > 250       |                                     |
| 1-Tetradecanol                    | 32.72                                    | 0.0703    | 39.5 to 289       |                                     |
| Tetraethylene glycol              | 45(25)                                   |           | − 6 to 328        | 44.9(25)                            |
| Tetraethyl lead                   | 30.50                                    | 0.0969    | − 136 to > 85     |                                     |
| Tetraethylsilane                  | 25.22                                    | 0.1079    | − 82 to 154.7     |                                     |
| Tetraethyl silicate               | 23.63                                    | 0.0979    | − 82.5 to 169     |                                     |
| Tetrahydrofuran                   | 26.5(25)                                 |           | − 108.5 to 65     | 0.605(0), 0.460(25), 0.359(50)      |
| 2,5-Tetrahydrofuran dimethanol    |                                          |           | < − 50 to 265     | 225(25)                             |
| Tetrahydro-2-furanmethanol        | 39.96                                    | 0.1008    | < − 80 to 178     | 6.24(20)                            |
| 1,2,3,4-Tetrahydronaphthalene     | 35.55                                    | 0.0954    | − 35.8 to 207.6   | 2.202(20), 2.003(25)                |
| Tetrahydropyran                   |                                          |           | − 45 to 88        | 0.826(20), 0.764(25)                |

**TABLE 5.16** Viscosity and Surface Tension of Various Organic Substances (*Continued*)

| Substance                                   | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |           | Liquid range, °C | Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|---------------------------------------------|-----------------------------------------------------|-----------|------------------|-----------------------------------------------------------|
|                                             | <i>a</i>                                            | <i>b</i>  |                  |                                                           |
| Tetrahydropyran-2-methanol                  | 34.1(25)                                            |           | − 70 to 187      | 11.0(20)                                                  |
| Tetrahydrothiophene-1,1-dioxide (sulfolane) | 35.5(30)                                            |           | 27.6 to 287.3    | 9.87(30), 6.280(50), 3.818(75)                            |
| Tetrahydrothiophene oxide                   |                                                     |           |                  | 52(30), 19(80)                                            |
| Thiacyclohexane                             | 36.06(20)                                           | 33.74(40) |                  |                                                           |
| Thiacyclopentane                            | 38.44                                               | 0.1342    |                  | 1.042(20), 0.971(25)                                      |
| 2,2'-Thiodiethanol                          | 53.8(20)                                            |           | − 10.2 to 282    | 65.2(20)                                                  |
| Thiophene                                   | 34.00                                               | 0.1328    | − 39.4 to 84     | 0.871(0), 0.662(20), 0.353(82)                            |
| Thymol                                      | 33.95                                               | 0.0821    | 49 to 232        |                                                           |
| Toluene                                     | 30.90                                               | 0.1189    | − 94.9 to 110.6  | 0.623(15), 0.523(30), 0.424(50)                           |
| <i>p</i> -Toluenesulfonyl chloride          | 42.41                                               | 0.0903    | 67 to > 134      |                                                           |
| <i>o</i> -Toluidine                         | 42.87                                               | 0.1094    | − 16.5 to 200    | 5.195(15), 4.39(20)                                       |
| <i>m</i> -Toluidine                         | 40.33                                               | 0.0979    | − 31 to 203      | 4.418(15), 2.741(30)                                      |
| <i>p</i> -Toluidine                         | 39.58                                               | 0.0957    | 43.8 to 200      | 1.945(45), 1.557(60)                                      |
| <i>m</i> -Tolunitrile                       | 38.85                                               | 0.1013    | − 23 to 210      |                                                           |
| <i>p</i> -Tolunitrile                       | 39.79                                               | 0.1100    | 29.5 to 85       |                                                           |
| Tribenzylamine                              | 42.41                                               | 0.0953    | 91-94 to bp      |                                                           |
| Tribromomethane                             | 48.14                                               | 0.1308    | 8.1 to 149.6     | 2.152(15), 1.741(30), 1.367(50)                           |
| 1,2,3-Tribromopropane                       | 47.99                                               | 0.1267    | 16.5 to 220      |                                                           |
| Tributylamine                               | 26.47                                               | 0.0831    | − 70 to 216      | 1.35(25)                                                  |
| Tributyl borate                             | 26.2(20)                                            | 25.8(25)  | < − 70 to 234    | 1.776(20), 1.601(25)                                      |
| Tributyl phosphite                          | 27.57                                               | 0.0865    | up to > 125      | 1.9(25)                                                   |
| Tributyl phosphate                          | 28.71                                               | 0.0666    | − 79 to 289      | 11.1(15), 3.39(25)                                        |
| Trichloroacetaldehyde                       | 27.66                                               | 0.1197    | − 57.5 to 97.8   |                                                           |
| Trichloroacetic acid                        | 35.4                                                | 0.0895    | 57.5 to 196.5    |                                                           |
| 1,1,1-Trichloroethane                       | 28.28                                               | 0.1242    | − 30.4 to 74     | 0.903(15), 0.725(30), 0.578(50)                           |
| 1,1,2-Trichloroethane                       | 37.40                                               | 0.1351    | − 37 to 114      | 0.119(20), 0.110(25)                                      |
| Trichloroethylene                           | 29.5(20)                                            | 28.8(25)  | − 84.8 to 87     | 0.703(0), 0.545(25), 0.444(50)                            |
| Trichlorofluoromethane                      | 18(25)                                              |           | − 111 to 23.8    | 0.740(− 25), 0.539(0)                                     |
| 2,4,6-Trichlorophenol                       | 43.13                                               | 0.0955    | 69 to 246        |                                                           |
| 1,2,3-Trichloropropane                      | 37.8(20)                                            | 37.05(25) | − 14.7 to 157    |                                                           |
| Trichlorosilane                             | 20.43                                               | 0.1076    | − 127 to 32      | 0.332(20), 0.316(25)                                      |
| $\alpha,\alpha,\alpha$ -Trichlorotoluene    |                                                     |           | − 5 to 223       | 3.07(10), 2.55(17)                                        |
| 1,1,2-Trichloro-1,2,2-trifluoroethane       | 17.75(20)                                           | 16.56(30) | − 35 to 47.7     | 0.711(20), 0.627(30)                                      |
| Tridecane                                   | 27.73                                               | 0.0872    | − 5 to 235       | 2.909(0), 1.724(25), 1.129(50)                            |
| 1-Tridecene                                 | 28.01                                               | 0.0884    | − 13 to 232.8    |                                                           |
| Triethanolamine                             |                                                     |           | 20.5 to 335.4    | 609(25), 114(50), 31.5(75)                                |
| Triethylamine                               | 22.70                                               | 0.0992    | − 114.7 to 88.8  | 0.455(0), 0.347(25), 0.273(50)                            |
| Triethylene glycol                          | 47.33                                               | 0.0880    | − 7 to 285       | 49.0(20), 8.5(60)                                         |
| Triethyl phosphate                          | 31.81                                               | 0.0928    | − 56 to 215      | 1.684(40), 1.376(55)                                      |
| Triethyl phosphite                          | 25.73                                               | 0.0878    | up to 156        | 0.72(25)                                                  |
| Trifluoroacetic acid                        | 15.64                                               | 0.1844    | − 15.3 to 73     | 0.926(20), 0.808(25), 0.571(50)                           |
| 2,2,2-Trifluoroethanol                      | 20.6(33)                                            |           | − 43.5 to 74     | 1.996(20)                                                 |
| Trimethylamine                              | 16.24                                               | 0.1133    | − 117 to 2.9     | 0.321(− 33.5)                                             |
| 1,2,3-Trimethylbenzene                      | 30.91                                               | 0.1040    | − 25.4 to 176.1  |                                                           |
| 1,2,4-Trimethylbenzene                      | 31.76                                               | 0.1025    | − 43.9 to 169    | 0.894(15), 0.730(30)                                      |
| 1,3,5-Trimethylbenzene                      | 29.79                                               | 0.0897    | − 44.7 to 165    | 1.154(20)                                                 |
| 2,2,3-Trimethylbutane                       | 20.70                                               | 0.0973    | − 24.9 to 80.9   | 0.579(20)                                                 |

TABLE 5.16 Viscosity and Surface Tension of Various Organic Substances (Continued)

| Substance                                | Surface tension,<br>mN · m <sup>-1</sup> |           | Liquid range, °C | Viscosity, mN · s · m <sup>-2</sup> |
|------------------------------------------|------------------------------------------|-----------|------------------|-------------------------------------|
|                                          | <i>a</i>                                 | <i>b</i>  |                  |                                     |
| <i>cis</i> -1,3,5-Trimethylcyclohexane   |                                          |           |                  | 0.632(20), 0.558(30)                |
| <i>trans</i> -1,3,5-Trimethylcyclohexane |                                          |           | − 107.4 to 140.5 | 0.714(20), 0.624(30)                |
| Trimethylene sulfide                     | 36.3(20)                                 | 35.0(30)  | − 73.2 to 95     | 0.638(20), 0.607(25)                |
| 3,5,5-Trimethyl-1-hexanol                |                                          |           | < − 70 to 194    | 11.06(25)                           |
| 2,2,3-Trimethylpentane                   | 22.46                                    | 0.0895    | − 112.3 to 110   | 0.598(20)                           |
| 2,2,4-Trimethylpentane                   | 20.55                                    | 0.0888    | − 107.4 to 99.2  | 0.502(20)                           |
| Trimethyl phosphite                      | 27.18(20)                                | 24.88(40) | − 78 to 112      | 0.61(20)                            |
| 2,4,6-Trimethylpyridine                  |                                          |           | − 46 to 171      | 1.498(20)                           |
| Triphenylamine                           | 46.2                                     | 0.0955    | 125 to 348       |                                     |
| Triphenyl phosphite                      |                                          |           | 22 to 360        | 6.95(45)                            |
| Tripropylamine                           | 24.58                                    | 0.0878    | − 93.5 to 158    |                                     |
| Tripropylene glycol                      | 34(25)                                   |           | up to 273        | 56.1(25)                            |
| Tripropylene glycol butyl ether          | 28.8(25)                                 |           | up to 276        | 6.58(25)                            |
| Tripropylene glycol ethyl ether          | 28.2(25)                                 |           |                  | 5.17(25)                            |
| Tripropylene glycol isopropyl ether      | 27.4(25)                                 |           |                  | 7.7(25)                             |
| Tripropylene glycol methyl ether         | 30.0(25)                                 |           | − 42 to 242.4    | 5.96(25)                            |
| Tris( <i>m</i> -tolyl) phosphite         |                                          |           |                  | 37.55(15), 9.132(45), 5.075(65)     |
| Tris( <i>p</i> -tolyl) phosphite         |                                          |           |                  | 35.52(15), 8.794(45), 5.017(65)     |
| Tri- <i>o</i> -tolyl phosphate           | 40.9(20)                                 |           | 11 to 410        | 38.8(35), 16.8(55)                  |
| Undecane                                 | 26.26                                    | 0.0901    | − 25.6 to 196    | 1.707(0), 1.098(25), 0.761(50)      |
| Vinyl acetate                            | 23.95(20)                                | 22.54(30) | − 93 to 73       | 0.421(20)                           |
| <i>o</i> -Xylene                         | 32.51                                    | 0.1101    | − 25.2 to 145    | 1.084(0), 0.760(25), 0.561(50)      |
| <i>m</i> -Xylene                         | 31.23                                    | 0.1104    | − 47.9 to 139    | 0.795(0), 0.581(25), 0.445(50)      |
| <i>p</i> -Xylene                         | 30.69                                    | 0.1074    | 13 to 138        | 0.603(25), 0.457(50), 0.359(75)     |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances

The temperature in degrees Celsius at which the dielectric constant and dipole moment were measured is shown in this table in parentheses after the value. In some cases, the dipole moment was determined with the substance dissolved in a solvent, and the solvent used is also shown in parentheses after the temperature.

The dielectric constant (permittivity) tabulated is the relative dielectric constant, which is the ratio of the actual electric displacement to the electric field strength when an external field is applied to the substance, which is the ratio of the actual dielectric constant to the dielectric constant of a vacuum. The table gives the static dielectric constant  $\epsilon$ , measured in static fields or at relatively low frequencies where no relaxation effects occur.

The dipole moment is given in debye units D. The conversion factor to SI units is  $1 \text{ D} = 3.33564 \times 10^{-30} \text{ C} \cdot \text{m}$ .

Alternative names for entries are listed in Table 1.15 at the bottom of each double page.

#### List of Abbreviations

|                   |            |
|-------------------|------------|
| B, benzene        | g, gas     |
| C, $\text{CCl}_4$ | Hx, hexane |
| cHex, cyclohexane | lq, liquid |
| D, 1,4-dioxane    |            |

| Substance                                           | Dielectric constant, $\epsilon$   | Dipole moment, D             |
|-----------------------------------------------------|-----------------------------------|------------------------------|
| Acetaldehyde                                        | 21.8 (10), 21.0 (18)              | 2.75                         |
| Acetaldehyde oxime                                  | 4.70 (25)                         | 0.830 (20, lq), 0.90 (25, B) |
| Acetamide                                           | 67.6 (91)                         | 3.76                         |
| Acetanilide                                         |                                   | 3.65 (25, B)                 |
| Acetic acid                                         | 6.20 (20)                         | 1.70                         |
| Acetic anhydride                                    | 23.3 (0), 22.45 (20)              | 2.8                          |
| Acetone                                             | 21.0 (20), 20.7 (25), 17.6 (56)   | 2.88                         |
| Acetonitrile                                        | 36.64 (20), 26.6 (82)             | 3.924                        |
| Acetophenone                                        | 17.44 (25), 8.64 (202)            | 3.02                         |
| ( $\pm$ )- <i>erythro</i> -2-Acetoxy-2-bromo-butane | 7.268 (25)                        |                              |
| ( $\pm$ )- <i>threo</i> -2-Acetoxy-2-bromobutane    | 7.414 (25)                        |                              |
| Acetyl bromide                                      | 16.2 (20)                         | 2.43 (20, B)                 |
| Acetyl chloride                                     | 16.9 (2), 15.8 (22)               | 2.72                         |
| Acetylene                                           | 2.484 (−77)                       |                              |
| Acrylonitrile                                       | 33.0 (20)                         | 3.87                         |
| Allene                                              | 2.025 (−4)                        |                              |
| Allylamine                                          |                                   | 1.2                          |
| Allyl alcohol                                       | 19.7 (20)                         | 1.61                         |
| Allyl isocyanate                                    | 15.15 (15)                        |                              |
| Allyl isothiocyanate                                | 17.2 (18)                         | 3.2 (20, B)                  |
| Allyl nitrite                                       | 9.12 (25)                         |                              |
| 2-Aminoethanol                                      | 31.94 (20), 37.72 (25)            | 2.59 (25, D)                 |
| 2-(2-Aminoethylamino)ethanol                        | 21.81 (20)                        |                              |
| <i>N</i> -(2-Aminoethyl)-1,2-ethane-diamine         | 12.62 (20)                        | 1.9                          |
| Aniline                                             | 7.06 (20), 5.93 (70)              | 1.13                         |
| Benzaldehyde                                        | 19.7 (0), 17.85 (20)              | 3.0                          |
| Benzaldehyde oxime (mp 30) (mp 128)                 | 3.8 (20)                          | 1.2 (25, B)<br>1.5 (25, B)   |
| Benzamide                                           |                                   | 3.42 (25, B)                 |
| Benzene                                             | 2.292(15), 2.283 (20), 2.274 (25) | 0                            |
| Benzeneacetonitrile                                 | 17.87 (26)                        | 3.5                          |
| Benzenesulfonyl chloride                            | 28.90 (50)                        | 4.50 (20, B)                 |
| Benzenethiol                                        | 4.38 (25), 4.26 (30)              | 1.13 (25, lq), 1.19 (20, B)  |
| Benzonitrile                                        | 25.9 (20), 24.0 (40)              | 4.18                         |
| Benzophenone                                        | 14.60 (18), 11.4 (50)             | 3.09 (50, lq), 2.98 (25, B)  |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                        | Dielectric constant, $\epsilon$   | Dipole moment, D             |
|----------------------------------|-----------------------------------|------------------------------|
| Benzoyl bromide                  | 21.33 (20), 20.74 (25)            | 3.40 (20, B)                 |
| Benzoyl chloride                 | 29.0 (0), 23 (23)                 | 3.16 (25, B)                 |
| Benzoyl fluoride                 | 22.7 (20)                         |                              |
| Benzyl acetate                   | 5.1 (21), 5.34 (930)              | 1.80 (25, B)                 |
| Benzyl alcohol                   | 13.0 (20), 11.92 (30), 9.5 (70)   | 1.71                         |
| Benzylamine                      | 5.5 (1), 5.18 (20)                | 1.15 (20, lq), 1.38 (25, B)  |
| Benzyl benzoate                  | 5.26 (30)                         | 2.06 (30, B)                 |
| Benzyl chloride                  | 7.0 (13), 6.85 (25)               | 1.83 (20, B)                 |
| Benzylethylamine                 | 4.3 (20)                          |                              |
| Benzyl ethyl ether               | 3.90 (25)                         |                              |
| Benzyl formate                   | 6.34 (30)                         |                              |
| N-Benzylmethylamine              | 4.4 (19)                          |                              |
| Biphenyl                         | 2.53 (75)                         | 0                            |
| Bis(2-aminoethyl)amine           | 12.62 (20)                        |                              |
| Bis(2-chloroethyl) ether         | 21.20 (20)                        | 2.6                          |
| Bis(3-chloropropyl) ether        | 10.10 (20)                        |                              |
| Bis(2-ethoxyethyl) ether         |                                   | 1.92 (25, B)                 |
| Bis(2-hydroxyethyl) ether        | 31.69 (20)                        | 2.31 (20, B)                 |
| Bis(2-hydroxyethyl)sulfide       | 28.61 (20)                        |                              |
| Bis(2-hydroxypropyl) ether       | 20.38 (20)                        |                              |
| Bis(2-methoxyethyl) ether        | 7.23 (25)                         |                              |
| ( $\pm$ )-Bornyl acetate         | 4.6 (21)                          | 1.89 (22)                    |
| 3-Bromoaniline                   | 13.0 (20)                         | 2.67 (20, B)                 |
| 4-Bromoaniline                   | 7.06 (30)                         | 2.88 (25, B)                 |
| 2-Bromoanisole                   | 8.96 (30)                         |                              |
| 4-Bromoanisole                   | 7.40 (30)                         |                              |
| Bromobenzene                     | 5.45 (20), 5.40 (25)              | 1.70                         |
| 1-Bromobutane                    | 7.88 (– 10), 7.32 (10), 7.07 (20) | 2.08                         |
| ( $\pm$ )-2-Bromobutane          | 8.64 (25)                         | 2.23                         |
| 2-Bromobutanoic acid             | 7.2 (20)                          |                              |
| cis-2-Bromo-2-butene             | 5.38 (20)                         |                              |
| trans-2-Bromo-2-butene           | 6.76 (20)                         |                              |
| 1-Bromo-2-chlorobenzene          | 6.80 (20)                         | 2.15 (20, B)                 |
| 1-Bromo-3-chlorobenzene          | 4.58 (20)                         | 1.52 (22, B)                 |
| 1-Bromo-4-chlorobenzene          |                                   | 0.1 (25, B)                  |
| 1-Bromo-2-chloroethane           | 7.41 (10)                         | 1.09                         |
| cis-1-Bromo-2-chloroethene       | 7.31 (17)                         |                              |
| trans-1-Bromo-2-chloroethene     | 2.50 (17)                         |                              |
| Bromochlorodifluoromethane       | 3.92 (– 150)                      |                              |
| Bromochloromethane               | 7.79                              | 1.66 (25, B)                 |
| 3-Bromo-1-chloro-2-methylpropane | 8.90 (30)                         |                              |
| Bromocyclohexane                 | 11 (– 65), 8.003(30)              | 1.08 (25, lq), 2.3 (25, B)   |
| 1-Bromodecane                    | 4.75 (1), 4.44 (25)               | 2.08 (20, lq), 1.90 (25, lq) |
| Bromodichloromethane             |                                   | 1.31 (25, B)                 |
| 1-Bromododecane                  | 4.07 (25)                         | 2.01 (25, lq), 1.89 (25, B)  |
| Bromoethane                      | 13.6 (– 60), 9.39 (20), 9.01 (25) | 2.03 (g), 2.04 (20, lq)      |
| 1-Bromo-2-ethoxypentane          | 6.45 (25)                         | 2.32 (25, B)                 |
| 2-Bromo-3-ethoxypentane          | 6.40 (25)                         | 2.07 (25, B)                 |
| 3-Bromo-2-ethoxypentane          | 8.24 (25)                         | 2.15 (25, B)                 |
| 1-Bromo-2-ethylbenzene           | 5.55 (25)                         |                              |
| 1-Bromo-3-ethylbenzene           | 5.56 (25)                         |                              |
| 1-Bromo-4-ethylbenzene           | 5.42 (25)                         |                              |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                     | Dielectric constant, $\epsilon$     | Dipole moment, D             |
|-------------------------------|-------------------------------------|------------------------------|
| Bromoethylene                 | 5.63 (5), 4.78 (25)                 | 1.42                         |
| 1-Bromo-2-fluorobenzene       | 4.72 (25)                           |                              |
| 1-Bromo-3-fluorobenzene       | 4.85 (25)                           |                              |
| 1-Bromo-4-fluorobenzene       | 2.60 (25)                           |                              |
| Bromoform                     | 4.39 (20)                           | 1.00, 0.92 (25, lq)          |
| 1-Bromoheptane                | 5.33 (25), 4.48 (90)                | 2.17, 2.02 (20, lq)          |
| 2-Bromoheptane                | 6.46 (22)                           | 2.08 (20, B)                 |
| 3-Bromoheptane                | 6.93 (22)                           | 2.06 (20, B)                 |
| 4-Bromoheptane                | 6.81 (22)                           | 2.06 (20, B)                 |
| 1-Bromohexadecane             | 3.71 (25)                           | 1.98 (20, lq), 1.96 (25, C)  |
| 1-Bromohexane                 | 6.30 (1), 5.82 (25)                 | 2.06 (20, lq)                |
| Bromomethane                  | 9.82 (0), 9.71 (3), 1.0068 (100, g) | 1.82                         |
| (Bromomethyl)benzene          | 6.658 (20)                          |                              |
| 1-Bromo-3-methylbutane        | 8.04 (– 56), 6.33 (18)              | 1.95 (20, B)                 |
| 2-Bromo-2-methylbutane        | 9.21 (25)                           |                              |
| 2-Bromo-3-methylbutanoic acid | 6.5 (20)                            |                              |
| 1-Bromo-2-methylpropane       | 10.98 (20), 7.2 (25)                | 1.92 (25, lq), 1.99 (20, B)  |
| 2-Bromo-2-methylpropane       | 10.98 (20)                          |                              |
| 1-Bromonaphthalene            | 5.83 (25), 5.12 (20)                | 1.29 (25, lq)                |
| 3-Bromonitrobenzene           | 20.2 (55)                           |                              |
| 1-Bromononane                 | 5.42 (– 20), 4.74 (25)              | 1.95 (25, lq)                |
| 1-Bromooctane                 | 6.35 (– 50)                         | 1.99 (20, lq), 1.88 (25, lq) |
| 1-Bromopentadecane            | 3.9 (20)                            |                              |
| 1-Bromopentane                | 9.9 (– 90), 6.32 (25)               | 2.20                         |
| 3-Bromopentane                | 8.37 (25)                           |                              |
| 1-Bromopropane                | 8.09 (20)                           | 2.18                         |
| 2-Bromopropane                | 9.46 (20)                           | 2.21                         |
| 2-Bromopropanoic acid         | 11.0 (21)                           |                              |
| 3-Bromopropene                | 7.0 (20)                            | 1.9                          |
| 2-Bromopyridine               | 23.18 (25)                          |                              |
| 1-Bromotetradecane            | 3.84 (25)                           | 1.92 (20, lq), 1.83 (25, lq) |
| <i>o</i> -Bromotoluene        | 4.64 (20), 4.28 (58)                | 1.45 (20, B)                 |
| <i>m</i> -Bromotoluene        | 5.566 (20), 5.36 (58)               | 1.77 (20, B)                 |
| <i>p</i> -Bromotoluene        | 5.503 (20), 5.49 (58)               | 1.95 (20, B)                 |
| Bromotrichloromethane         | 2.40 (20)                           |                              |
| Bromotrifluoromethane         | 3.73 (– 150)                        | 0.65                         |
| 1-Bromoundecane               | 4.73 (– 9)                          |                              |
| 1,3-Butadiene                 | 2.050 (– 8)                         | 0.403                        |
| Butanal                       | 13.45 (25)                          | 2.72                         |
| Butane                        | 1.7697 (22)                         | 0                            |
| 1,2-Butanediol                | 22.4 (25)                           |                              |
| 1,3-Butanediol                | 28.8 (25)                           |                              |
| 1,4-Butanediol                | 33 (15), 31.9 (25), 30 (38)         | 4.07                         |
| 1,3-Butanediol dinitrate      | 18.85 (20)                          |                              |
| 2,3-Butanediol dinitrate      | 28.85 (20)                          |                              |
| 1,3-Butanedione               | 4.04 (25)                           |                              |
| Butanenitrile                 | 24.83 (20)                          | 4.07                         |
| Butanesulfonyl chloride       |                                     | 3.94 (25, D)                 |
| 1,2,3,4-Butanetetrol          | 28.2 (120)                          |                              |
| 1-Butanethiol                 | 5.20 (15), 5.07 (25), 4.59 (50)     | 1.54 (25, lq or B)           |
| 2-Butanethiol                 | 5.645 (15)                          |                              |
| Butanoic acid                 | 2.97 (20)                           | 1.65 (30, B)                 |



**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                            | Dielectric constant, $\epsilon$ | Dipole moment, D            |
|--------------------------------------|---------------------------------|-----------------------------|
| Butanoic anhydride                   | 12.8 (20)                       |                             |
| 1-Butanol                            | 17.84 (20), 8.2 (118)           | 1.66                        |
| ( $\pm$ )-2-Butanol                  | 17.26 (20), 16.6 (25)           | 1.66 (30, B)                |
| 2-Butanone                           | 18.56 (20), 15.3 (60)           | 2.78                        |
| 2-Butanone oxime                     | 3.4 (20)                        |                             |
| <i>trans</i> -2-Butenal              |                                 | 3.67                        |
| 1-Butene                             | 2.2195 (– 53), 1.0032 (20, g)   | 0.438                       |
| <i>cis</i> -2-Butene                 | 1.960 (23)                      | 0.253                       |
| <i>trans</i> -2-Butene               |                                 | 0                           |
| 3-Butenenitrile                      | 28.1 (20)                       | 4.53                        |
| 2-Butoxyethanol                      | 9.43 (25)                       | 2.08 (25, B)                |
| Butoxyethyne                         | 6.62 (25)                       | 2.05 (25, lq)               |
| <i>N</i> -Butylacetamide             | 104.0 (20)                      |                             |
| <i>N-sec</i> -Butylacetamide         | 100.0 (100)                     |                             |
| Butyl acetate                        | 6.85 (– 73), 5.07 (20)          | 1.86 (22, B)                |
| <i>sec</i> -Butyl acetate            | 5.135 (20)                      | 1.9                         |
| <i>tert</i> -Butyl acetate           | 5.672 (20)                      | 1.91 (25, B)                |
| <i>tert</i> -Butylacetic acid        | 2.85 (23)                       |                             |
| Butyl acrylate                       | 5.25 (28)                       |                             |
| Butylamine                           | 4.71 (20)                       | 1.00                        |
| <i>sec</i> -Butylamine               | 4.4 (21)                        | 1.28 (25, B)                |
| <i>tert</i> -Butylamine              |                                 | 1.29 (25, B)                |
| Butylbenzene                         | 2.36 (20)                       | 0                           |
| <i>sec</i> -Butylbenzene             | 2.36 (20)                       | 0                           |
| <i>tert</i> -Butylbenzene            | 2.36 (20)                       | 0.83                        |
| Butyl butanoate                      | 4.39 (25)                       |                             |
| Butyl ethyl ether                    |                                 | 1.24                        |
| Butyl formate                        | 6.10 (30), 2.43 (80)            | 2.08 (26, lq), 2.03 (25, B) |
| Butyl isocyanate                     | 12.29 (20)                      |                             |
| Butyl methyl ether                   |                                 | 1.25 (25, B)                |
| 2- <i>tert</i> -Butyl-4-methylphenol |                                 | 1.31 (20, B)                |
| Butyl nitrate                        | 13.10 (20)                      | 2.99 (20, B)                |
| <i>tert</i> -Butyl nitrite           | 11.47 (25)                      |                             |
| Butyl oleate                         | 4.00 (25)                       |                             |
| <i>N</i> -Butylpropanamide           | 100.6 (25)                      |                             |
| Butyl propanoate                     | 4.838 (20)                      | 1.79 (23, B)                |
| 4- <i>tert</i> -Butylpyridine        |                                 | 2.87 (25, C)                |
| Butylsilane                          | 2.537 (20)                      |                             |
| Butyl stearate                       | 3.11 (30)                       | 1.88 (24, B)                |
| Butyl trichloroacetate               | 7.480 (20)                      |                             |
| Butyl vinyl ether                    |                                 | 1.25 (25, Hx)               |
| 4-Butyrolactone                      | 39.0 (20)                       | 4.27                        |
| Camphor                              | 11.35 (20)                      | 2.91 (20, B), 3.10 (25, B)  |
| Carbon disulfide                     | 3.0 (– 112), 2.64 (20)          | 0                           |
| Carbon tetrachloride                 | 2.24 (20), 2.228 (25)           | 0                           |
| Carbon tetrafluoride                 | 1.0006 (25, g)                  | 0                           |
| D-(+)-Carvone                        | 11 (22)                         | 2.8 (15, B)                 |
| Chloroacetic acid                    | 20 (20), 12.35 (65)             | 2.31 (30, B)                |
| <i>o</i> -Chloroaniline              | 13.40 (20)                      | 1.78 (20, B)                |
| <i>m</i> -Chloroaniline              | 13.3 (20)                       | 2.68 (20, B)                |
| <i>p</i> -Chloroaniline              |                                 | 2.99 (25, B)                |
| Chlorobenzene                        | 5.69 (20), 4.2 (120)            | 1.69                        |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                               | Dielectric constant, $\epsilon$    | Dipole moment, D            |
|-----------------------------------------|------------------------------------|-----------------------------|
| 2-Chloro-1,3-butadiene                  | 4.914 (20)                         |                             |
| 1-Chlorobutane                          | 9.07 (– 30), 7.276 (20)            | 2.05 (g), 2.0 (20, B)       |
| 2-Chlorobutane                          | 8.564 (20), 7.09 (30)              | 2.04 (g), 2.1 (20, B)       |
| Chlorocyclohexane                       | 10.9 (– 47), 7.951 (30)            | 2.2 (25, B)                 |
| Chlorodifluoromethane                   | 6.11 (24)                          | 1.42 (g)                    |
| 2-Chloro- <i>N,N</i> -dimethylacetamide | 39.2 (25)                          |                             |
| 1-Chlorododecane                        | 4.2 (20)                           | 2.11 (25, lq), 1.94 (20, B) |
| 1-Chloro-2,3-epoxypropane               | 25.6 (1), 22.6 (22)                | 1.8 (25, C)                 |
| Chloroethane                            | 1.013 (19, g), 9.45 (20)           | 2.05                        |
| 2-Chloroethanol                         | 25.80 (20), 13 (132)               | 1.78                        |
| (2-Chloro)ethylbenzene                  | 4.36 (25)                          |                             |
| (3-Chloro)ethylbenzene                  | 5.18 (25)                          |                             |
| (4-Chloro)ethylbenzene                  | 5.16 (25)                          |                             |
| 2-Chlorofluorobenzene                   | 6.10 (25)                          |                             |
| 3-Chlorofluorobenzene                   | 4.96 (25)                          |                             |
| 4-Chlorofluorobenzene                   | 3.34 (25)                          |                             |
| Chloroform                              | 4.807 (25), 4.31 (50)              | 1.04                        |
| 1-Chloroheptane                         | 5.52 (20)                          | 1.86 (22, B)                |
| 2-Chloroheptane                         | 6.52 (22)                          | 2.05 (22, B)                |
| 3-Chloroheptane                         | 6.70 (22)                          | 2.06 (22, B)                |
| 4-Chloroheptane                         | 6.54 (22)                          | 2.06 (22, B)                |
| 1-Chlorohexane                          | 6.104 (20)                         | 1.94 (20, B)                |
| 6-Chloro-1-hexanol                      | 21.6 (– 31)                        |                             |
| 1-Chloro-2-isocyanatoethane             | 29.1 (15)                          |                             |
| Chloromethane                           | 1.0069 (g), 12.6 (– 20), 10.0 (22) | 1.892                       |
| 1-Chloro-3-methylbutane                 | 7.63 (– 70), 6.05 (20)             | 1.94 (20, B)                |
| 2-Chloro-2-methylbutane                 | 12.31 (– 50)                       |                             |
| 4-Chloromethyl-1,3-dioxolan-2-one       | 97.5 (40)                          |                             |
| Chloromethyl methyl ether               |                                    | 1.88 (C)                    |
| (Chloromethyl)oxirane                   | 22.6 (20)                          | 1.8                         |
| 1-Chloro-2-methylpropane                | 7.87 (– 38), 7.027 (20)            | 2.00                        |
| 2-Chloro-2-methylpropane                | 10.95 (0), 9.66 (20)               | 2.13                        |
| 1-Chloronaphthalene                     | 5.04 (25)                          | 1.33 (25, lq), 1.52 (25, B) |
| <i>o</i> -Chloronitrobenzene            | 37.7 (50), 32 (80)                 | 4.64                        |
| <i>m</i> -Chloronitrobenzene            | 20.9 (50), 18 (80)                 | 3.73                        |
| <i>p</i> -Chloronitrobenzene            | 8.09 (120)                         | 2.83                        |
| 2-Chloro-2-nitropropane                 | 31.9 (– 23)                        |                             |
| 4-Chloro-3-nitrotoluene                 | 28.07 (28)                         |                             |
| 1-Chlorooctane                          | 5.05 (25)                          | 2.14 (25, lq)               |
| Chloropentafluoroethane                 |                                    | 0.52                        |
| 1-Chloropentane                         | 6.654 (20)                         | 2.16                        |
| <i>o</i> -Chlorophenol                  | 7.40 (21), 6.31 (25)               | 2.19                        |
| <i>m</i> -Chlorophenol                  | 6.255 (20)                         | 2.19 (25, B)                |
| <i>p</i> -Chlorophenol                  | 11.18 (41)                         | 2.11                        |
| 1-Chloropropane                         | 8.59 (20)                          | 2.05                        |
| 2-Chloropropane                         | 9.82 (20)                          | 2.17                        |
| 3-Chloro-1,2-propanediol                | 31.0 (20)                          |                             |
| 3-Chloro-1,2-propanediol dinitrate      | 17.50 (20)                         |                             |
| 3-Chloro-1-propanol                     | 36.0 (– 58)                        |                             |
| 1-Chloro-2-propanol                     | 59.0 (– 120)                       |                             |
| 1-Chloro-2-propanone                    | 30 (19)                            | 2.22 (g), 2.37 (20, Hx)     |
| 2-Chloro-1-propene                      | 8.92 (26)                          | 1.647                       |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                 | Dielectric constant, $\epsilon$   | Dipole moment, D            |
|-------------------------------------------|-----------------------------------|-----------------------------|
| 3-Chloro-1-propene                        | 8.2 (20)                          | 1.94                        |
| 2-Chloropyridine                          | 27.32 (20)                        |                             |
| 4-Chlorothiophenol                        | 3.59 (65)                         |                             |
| <i>o</i> -Chlorotoluene                   | 4.72 (20), 4.2 (55)               | 1.56                        |
| <i>m</i> -Chlorotoluene                   | 5.76 (20), 5.0 (60)               | 1.77 (20, lq), 1.8 (22, B)  |
| <i>p</i> -Chlorotoluene                   | 6.25 (20), 5.6 (55)               | 2.21                        |
| Chlorotrifluoromethane                    | 1.0013 (29, g), 3.01 (– 150)      | 0.50                        |
| 2-Chloro-1-trifluoromethyl-5-nitrobenzene | 9.8 (30)                          |                             |
| 4-Chloro-1-trifluoromethyl-3-nitrobenzene | 12.8 (30)                         |                             |
| 3-Chloro-1,1,1-trifluoropropane           | 7.32 (22)                         |                             |
| Chlorotrimethylsilane                     |                                   | 2.09 (20, B)                |
| Cineole                                   | 4.57 (25)                         |                             |
| Cinnamaldehyde                            | 17 (20), 16.9 (24)                | 3.74                        |
| <i>o</i> -Cresol                          | 6.76 (25)                         | 1.45 (25, B)                |
| <i>m</i> -Cresol                          | 12.44 (25)                        | 1.61 (25, B)                |
| <i>p</i> -Cresol                          | 13.05 (25)                        | 1.54 (20, B)                |
| Crotonic acid                             |                                   | 2.13 (30, B)                |
| Cyanoacetic acid                          | 33.4 (4)                          |                             |
| Cyanoacetylene                            | 72.3 (19)                         | 3.724                       |
| 2-Cyanopyridine                           | 93.77 (30)                        |                             |
| 3-Cyanopyridine                           | 20.54 (50)                        |                             |
| 4-Cyanopyridine                           | 5.23 (80)                         |                             |
| Cyclobutanone                             | 14.27 (25)                        | 2.89                        |
| Cycloheptane                              | 2.078 (30)                        |                             |
| Cycloheptanone                            | 13.16 (25)                        |                             |
| 1,3-Cyclohexadiene                        | 2.68 (– 89)                       | 0.38 (20, B)                |
| 1,4-Cyclohexadiene                        | 2.211 (23)                        |                             |
| Cyclohexane                               | 2.05 (15), 2.02 (25)              | 0                           |
| Cyclohexanecarboxylic acid                | 2.6 (31)                          |                             |
| 1,4-Cyclohexanedione                      | 15.0 (25), 4.40 (78)              | 1.41                        |
| Cyclohexanethiol                          | 5.420 (25)                        |                             |
| Cyclohexanol                              | 16.40 (20), 15.0 (25), 7.24 (100) | 1.86 (25, C)                |
| Cyclohexanone                             | 20 (– 40), 16.1 (20)              | 2.87                        |
| Cyclohexanone oxime                       | 3.04 (89)                         | 0.83 (25, B)                |
| Cyclohexene                               | 2.6 (– 105), 2.218 (20)           | 0.332                       |
| Cyclohexylamine                           | 4.55 (20)                         | 1.22 (20, lq), 1.26 (20, B) |
| Cyclohexylbenzene                         |                                   | 0                           |
| Cyclohexylmethanol                        | 9.7 (60), 8.1 (80)                | 1.68 (20, B)                |
| Cyclohexyl nitrite                        | 9.33 (25)                         |                             |
| <i>o</i> -Cyclohexylphenol                | 3.97 (55)                         |                             |
| <i>p</i> -Cyclohexylphenol                | 4.42 (131)                        |                             |
| Cyclooctane                               | 2.116 (22)                        | 0                           |
| <i>cis</i> -Cyclooctene                   | 2.306 (23)                        |                             |
| Cyclopentane                              | 1.9687 (20)                       | 0                           |
| Cyclopentanecarbonitrile                  | 22.68 (20)                        |                             |
| Cyclopentanol                             | 25 (– 20), 18.5 (10)              | 1.72 (25, C)                |
| Cyclopentanone                            | 16 (– 51), 13.58 (25)             | 3.30                        |
| Cyclopentene                              | 2.083 (22)                        | 0.20                        |
| <i>p</i> -Cymene                          | 2.243 (20), 2.23 (25)             | 0                           |
| <i>cis</i> -Decahydronaphthalene          | 2.22 (20)                         | 0                           |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                     | Dielectric constant, $\epsilon$  | Dipole moment, D            |
|-----------------------------------------------|----------------------------------|-----------------------------|
| <i>trans</i> -Decahydronaphthalene            | 2.18 (20)                        | 0                           |
| Decamethylcyclopentasiloxane                  | 2.5 (20)                         |                             |
| Decamethyltetrasiloxane                       | 2.4 (20)                         | 0.79 (25, lq)               |
| Decane                                        | 1.991 (20), 1.844 (130)          | 0                           |
| 1-Decanol                                     | 8.1 (20)                         | 1.71 (20, B), 1.62 (25, B)  |
| 1-Decene                                      | 2.14 (20)                        | 0                           |
| <i>meso</i> -2,3-Diacetoxybutane              | 6.644 (25)                       |                             |
| Diallyl sulfide                               | 4.9 (20)                         | 1.33 (25, B)                |
| Dibenzofuran                                  | 3.0 (100)                        | 0.88 (25, B)                |
| Dibenzylamine                                 | 3.6 (20)                         | 0.97 (20, lq), 1.02 (20, B) |
| Dibenzyl decanedioate                         | 4.6 (25)                         |                             |
| Dibenzyl ether                                | 3.82 (20)                        | 1.39 (21, B)                |
| <i>o</i> -Dibromobenzene                      | 7.86 (20)                        | 2.13 (20, B)                |
| <i>m</i> -Dibromobenzene                      | 4.21 (20)                        | 1.5 (20, B)                 |
| <i>p</i> -Dibromobenzene                      | 2.57 (95)                        | 0                           |
| 1,2-Dibromobutane                             | 4.74 (20)                        |                             |
| 1,3-Dibromobutane                             | 9.14 (20)                        |                             |
| 1,4-Dibromobutane                             | 8.68 (30)                        | 2.16 (20, lq), 2.06 (20, B) |
| 2,3-Dibromobutane                             | 6.36 (20), 5.75 (25)             | 2.20                        |
| <i>meso</i> -2,3-Dibromobutane                | 6.245 (25)                       |                             |
| ( $\pm$ )-2,3-Dibromobutane                   | 5.758 (25)                       |                             |
| 1,2-Dibromodichloromethane                    | 2.54 (25)                        |                             |
| 1,2-Dibromodifluoromethane                    | 2.94 (0)                         | 0.66                        |
| 1,2-Dibromoethane                             | 4.96 (20), 4.78 (25), 4.09 (131) | 1.11                        |
| <i>cis</i> -1,2-Dibromoethylene               | 7.08 (25)                        |                             |
| <i>trans</i> -1,2-Dibromoethylene             | 2.88 (25)                        |                             |
| Dibromomethane                                | 7.77 (10)                        | 1.43                        |
| <i>cis</i> -1,2-Dibromoethylene               | 7.7 (0), 7.08 (25)               | 1.35 (B)                    |
| <i>trans</i> -1,2-Dibromoethylene             | 2.9 (0), 2.88 (25)               | 0                           |
| 1,2-Dibromoheptane                            | 3.8 (25)                         | 1.78 (25, D)                |
| 2,3-Dibromoheptane                            | 5.1 (25)                         | 2.15 (25, B)                |
| 3,4-Dibromoheptane                            | 4.7 (25)                         | 2.15 (25, B)                |
| <i>meso</i> -3,4-Dibromohexane                | 4.67 (25)                        |                             |
| ( $\pm$ )-3,4-Dibromohexane                   | 6.732 (25)                       |                             |
| 1,6-Dibromohexane                             | 8.52 (25)                        |                             |
| Dibromomethane                                | 7.77 (10), 6.7 (40)              | 1.43                        |
| 1,2-Dibromo-2-methylpropane                   | 4.1 (20)                         |                             |
| 1,2-Dibromopentane                            | 4.39 (25)                        |                             |
| ( $\pm$ )- <i>erythro</i> -2,3-Dibromopentane | 5.43 (25)                        |                             |
| ( $\pm$ )- <i>threo</i> -2,3-Dibromopentane   | 6.507 (25)                       |                             |
| 1,4-Dibromopentane                            | 9.05 (20)                        |                             |
| 1,5-Dibromopentane                            | 9.14 (30)                        |                             |
| 1,2-Dibromopropane                            | 4.60 (10), 4.3 (20)              | 1.13                        |
| 1,3-Dibromopropane                            | 9.48 (20)                        |                             |
| Dibromotetrafluoroethane                      | 2.34 (25)                        |                             |
| Dibutylamine                                  | 2.78 (20)                        | 1.06 (20, lq), 1.05 (20, B) |
| Dibutyl decanedioate                          | 4.54 (20)                        | 2.64 (25, B)                |
| Dibutyl ether                                 | 3.08 (20)                        | 1.18                        |
| Dibutyl maleate                               |                                  | 2.70 (25, B)                |
| Dibutyl <i>o</i> -phthalate                   | 6.58 (20), 6.436 (30), 5.99 (45) | 2.97 (20, lq), 2.85 (30, B) |
| Dibutyl sulfide                               | 4.29 (25)                        | 1.6                         |
| Dichloroacetic acid                           | 8.33 (20), 7.8 (61)              |                             |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                       | Dielectric constant, $\epsilon$       | Dipole moment, D            |
|-------------------------------------------------|---------------------------------------|-----------------------------|
| Dichloroacetic anhydride                        | 15.8 (25)                             |                             |
| 1,1,-Dichloroacetone                            | 14.6 (20)                             |                             |
| <i>o</i> -Dichlorobenzene                       | 10.12 (20), 9.93 (25), 7.10 (90)      | 2.50                        |
| <i>m</i> -Dichlorobenzene                       | 5.02 (20), 5.04 (25), 4.22 (90)       | 1.72                        |
| <i>p</i> -Dichlorobenzene                       | 2.394 (55)                            | 0                           |
| 1,2-Dichlorobutane                              | 7.74 (25)                             |                             |
| 1,4-Dichlorobutane                              | 9.30 (35)                             | 2.22                        |
| Dichlorodifluoromethane                         | 3.50 (– 150), 2.13 (29)               | 0.51                        |
| 4-Chloro-1,3-dioxalan-2-one                     | 62.0 (40)                             |                             |
| 4,5-Dichloro-1,3-dioxalan-2-one                 | 31.8 (40)                             |                             |
| 1,1-Dichloroethane                              | 10.10 (20)                            | 2.06                        |
| 1,2-Dichloroethane                              | 12.7 (– 10), 10.42 (20)               | 1.48                        |
| 1,1-Dichloroethylene                            | 4.60 (20), 4.60 (25)                  | 1.34                        |
| <i>cis</i> -1,2-Dichloroethylene                | 9.20 (25)                             | 1.90                        |
| <i>trans</i> -1,2-Dichloroethylene              | 2.14 (20)                             | 0                           |
| 2,2'-Dichloroethyl ether                        | 21.2 (20)                             | 2.61 (20, B)                |
| Dichlorofluoromethane                           | 5.34 (28)                             | 1.29 (g)                    |
| 1,6-Dichlorohexane                              | 8.60 (35)                             |                             |
| Dichloromethane                                 | 9.14 (20), 8.93 (25), 1.0065 (100, g) | 1.60                        |
| 1,3-Dichloroisopropyl nitrate                   | 13.28 (20)                            |                             |
| (Dichloromethyl)benzene                         | 6.9 (20)                              | 2.1                         |
| Dichloromethyl isocyanate                       | 7.36 (15)                             |                             |
| 1,2-Dichloro-2-methylpropane                    | 7.15 (23)                             |                             |
| 2,4-Dichloro-1-nitrobenzene                     | 13.06 (28)                            |                             |
| 1,1-Dichloro-1-nitroethane                      | 16.3 (30)                             |                             |
| 1,2-Dichloropentane                             | 6.89 (20)                             |                             |
| 1,5-Dichloropentane                             | 9.92 (25)                             |                             |
| 2,4-Dichlorophenol                              |                                       | 1.60 (25, B)                |
| 1,2-Dichloropropane                             | 8.37 (20), 8.93 (26), 7.90 (35)       | 1.87 (25, B)                |
| 1,3-Dichloropropane                             | 10.27 (30)                            | 2.08                        |
| 2,2-Dichloropropane                             | 11.37 (20)                            | 2.62                        |
| 1,1-Dichloro-2-propanone                        | 14 (20)                               |                             |
| 1,2-Dichlorotetrafluoroethane                   | 2.48 (0), 2.26 (25)                   | 0.53                        |
| 2,4-Dichlorotoluene                             | 5.68 (28)                             | 1.7                         |
| 2,6-Dichlorotoluene                             | 3.36 (28)                             |                             |
| 3,4-Dichlorotoluene                             | 9.39 (28)                             | 3.0                         |
| Diethanolamine                                  | 25.75 (20)                            | 2.84 (25, B)                |
| 1,1-Diethoxyethane                              | 3.80 (25)                             | 1.08                        |
| 1,2-Diethoxyethane                              | 3.90 (20)                             | 1.99 (20, B), 1.65 (25, B)  |
| Diethoxymethane                                 | 2.527 (20)                            |                             |
| <i>N,N</i> -Diethylacetamide                    | 32.1 (20)                             |                             |
| <i>N,N</i> -Diethylacetoacetamide               | 40.8 (25)                             |                             |
| Diethylamine                                    | 3.680 (20)                            | 0.92                        |
| <i>N,N</i> -Diethylaniline                      | 5.5 (19)                              | 1.40 (20, lq), 1.80 (20, B) |
| Diethyl carbonate                               | 2.82 (24)                             | 1.10                        |
| <i>N,N</i> -Diethyl- <i>N',N'</i> -dimethylurea | 17.89 (25)                            |                             |
| Diethyl decanedioate                            | 5.0 (30)                              | 2.38 (20, lq), 2.52 (20, B) |
| Diethylene glycol                               | 3.182 (20)                            | 2.3                         |
| Diethylene glycol diethyl ether                 | 5.70                                  |                             |
| Diethyl ether                                   | 4.267 (20), 3.97 (40)                 | 1.15                        |
| Diethyl ethyl phosphonate                       | 11.00 (15), 9.86 (45)                 | 2.95 (32, lq), 2.91 (20, C) |
| <i>N,N</i> -Diethylformamide                    | 29.6 (20)                             |                             |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                            | Dielectric constant, $\epsilon$ | Dipole moment, D            |
|--------------------------------------|---------------------------------|-----------------------------|
| Diethyl fumarate                     | 6.56 (23)                       | 2.40 (20, B)                |
| Diethyl glutarate                    | 6.7 (30)                        | 2.46 (30, lq)               |
| Diethyl glycol                       | 31.82 (20)                      |                             |
| Di(2-ethylhexyl) <i>o</i> -phthalate | 5.3 (20), 4.91 (35), 4.77 (45)  | 2.8                         |
| Diethyl maleate                      | 8.58 (23), 7.56 (25)            | 2.56 (25, B)                |
| Diethyl methanephosphate             | 13.405 (40)                     |                             |
| Diethyl 1,3-propanedioate (malonate) | 8.03 (25), 7.55 (31)            | 2.49 (20, lq), 2.54 (25, B) |
| Diethyl nonanedioate                 | 5.13 (30)                       |                             |
| Diethyl oxalate                      | 8.266 (20)                      | 2.49 (20, D)                |
| Diethyl <i>o</i> -phthalate          | 7.34 (35), 7.13 (45)            | 2.8 (25, B)                 |
| Diethylsilane                        | 2.544 (20)                      |                             |
| Diethyl succinate                    | 6.098 (20)                      | 2.3                         |
| Diethyl sulfate                      | 29.2 (20)                       | 4.46 (25, D)                |
| Diethyl sulfide                      | 5.72 (25), 5.24 (50)            | 1.54                        |
| Diethyl sulfite                      | 15.6 (20), 14 (50)              |                             |
| Diethylzinc                          | 2.55 (20)                       | 0.62 (25, B)                |
| <i>o</i> -Difluorobenzene            | 13.38 (28)                      | 2.46                        |
| <i>m</i> -Difluorobenzene            | 5.01 (28)                       | 1.51                        |
| 1,1-Difluoroethane                   |                                 | 2.27                        |
| Difluoromethane                      | 53.74 (– 121)                   | 1.978                       |
| 2,3-Dihydropyran                     | 5.136 (35)                      |                             |
| 1,2-Dihydroxybenzene                 | 17.57 (115)                     | 2.60 (25, B)                |
| 1,3-Dihydroxybenzene                 | 13.55 (120)                     | 2.09 (44, B)                |
| 1,4-Dihydroxybenzene                 |                                 | 1.4 (44, B)                 |
| 1,2-Diiodobenzene                    | 5.7 (20), 5.41 (50)             | 1.70 (20, B)                |
| 1,3-Diiodobenzene                    | 4.3 (25), 4.11 (50)             | 1.22 (20, B)                |
| 1,4-Diiodobenzene                    | 2.88 (120)                      | 0.19 (20, B)                |
| <i>cis</i> -1,2-Diiodoethylene       | 4.46 (72)                       | 0.71 (B)                    |
| <i>trans</i> -1,2-Diiodoethylene     | 3.19 (77)                       | 0                           |
| Diiodomethane                        | 5.316 (25)                      | 1.08 (25, B)                |
| Diisobutylamine                      | 2.7 (22)                        | 1.10 (25, B)                |
| 1,6-Diisocyanatohexane               | 14.41 (15)                      |                             |
| Diisopentylamine                     | 2.5 (18)                        | 1.48 (30, B)                |
| Diisopentyl ether                    | 2.82 (20)                       | 0.98 (20, lq), 1.23 (25, B) |
| Diisopropylamine                     |                                 | 1.26 (25, B)                |
| Diisopropyl ether                    | 3.88 (25), 3.805 (30)           | 1.13                        |
| 1,2-Dimethoxybenzene                 | 4.45 (20), 4.09 (25)            | 1.32 (25, B)                |
| Dimethoxydimethylsilane              | 3.663 (25)                      |                             |
| 1,2-Dimethoxyethane                  | 7.60 (10), 7.30 (23.5)          | 1.71 (25, B)                |
| Dimethoxymethane                     | 2.644 (20)                      | 0.74                        |
| <i>N,N</i> -Dimethylacetamide        | 38.85 (21), 37.78 (25)          | 3.80                        |
| 2-Dimethylamino-2-methyl-1-propanol  | 12.36 (25)                      |                             |
| Dimethylamine                        | 6.32 (0), 5.26 (25)             | 1.01                        |
| <i>N,N</i> -Dimethylaniline          | 4.90 (25), 4.4 (70)             | 1.68                        |
| 2,4-Dimethylaniline                  | 4.9 (20)                        | 1.40 (25, B)                |
| 2,3-Dimethyl-1,3-butadiene           | 2.102 (20)                      |                             |
| <i>N,N</i> -Dimethylbutanamide       | 29.7 (20)                       |                             |
| 2,2-Dimethylbutane                   | 1.869 (20)                      | 0                           |
| 2,3-Dimethylbutane                   | 1.889 (20)                      | 0                           |
| 3,3-Dimethyl-2-butanone              | 12.73 (20)                      |                             |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                               | Dielectric constant, $\epsilon$    | Dipole moment, D           |
|-----------------------------------------|------------------------------------|----------------------------|
| 2,2-Dimethyl-1-butanol                  | 10.5 (20)                          |                            |
| Dimethyl carbonate                      | 3.087 (25)                         | 0.90                       |
| <i>cis</i> -1,2-Dimethylcyclohexane     | 2.06 (25)                          | 0                          |
| <i>trans</i> -1,2-Dimethylcyclohexane   | 2.04 (25)                          | 0                          |
| 1,1-Dimethylcyclopentane                |                                    | 0                          |
| Dimethyl disulfide                      | 9.6 (25)                           | 1.8                        |
| Dimethyl ether                          | 6.18 (– 15), 5.02 (25), 2.97 (110) | 1.30                       |
| <i>N,N</i> -Dimethylformamide           | 38.25 (20), 36.71 (25)             | 3.82 (25, B)               |
| 2,4-Dimethylheptane                     | 1.9 (20)                           | 0                          |
| 2,5-Dimethylheptane                     | 1.9 (20)                           | 0                          |
| 2,6-Dimethylheptane                     | 2 (20)                             | 0                          |
| 2,6-Dimethyl-4-heptanone                | 9.91 (20)                          | 2.66 (25, C)               |
| 2,2-Dimethylhexane                      | 1.95 (20)                          | 0                          |
| 2,5-Dimethylhexane                      | 1.96 (21)                          | 0                          |
| 3,3-Dimethylhexane                      | 1.96 (20)                          | 0                          |
| 3,4-Dimethylhexane                      | 1.98 (19)                          | 0                          |
| Dimethyl hexanedioate                   | 6.84 (20)                          | 2.28 (20, B)               |
| 1,3-Dimethylimidazolidin-2-one          | 37.60 (25)                         |                            |
| Dimethyl maleate                        |                                    | 2.48 (25, C)               |
| Dimethyl malonate                       | 9.82 (20)                          | 2.41 (20, B)               |
| Dimethyl methanephosphate               | 22.3 (20)                          |                            |
| <i>N,N</i> -Dimethyl methanesulfonamide | 80.4 (50)                          |                            |
| 1,2-Dimethylnaphthalene                 | 2.61 (25)                          | 0                          |
| 1,6-Dimethylnaphthalene                 | 2.73 (20)                          | 0                          |
| 4,4-Dimethyloxazolidine-2-one           | 39.2 (60)                          |                            |
| <i>N,N</i> -Dimethylpentanamide         | 26.4 (20)                          |                            |
| 2,2-Dimethylpentane                     | 1.915 (20)                         | 0                          |
| 2,3-Dimethylpentane                     | 1.929 (20)                         | 0                          |
| 2,4-Dimethylpentane                     | 1.902 (20)                         | 0                          |
| 3,3-Dimethylpentane                     | 1.942 (20)                         | 0                          |
| Dimethyl pentanedioate                  | 7.87 (20)                          |                            |
| 2,4-Dimethyl-3-pentanone                |                                    | 2.7                        |
| 2,3-Dimethylphenol                      | 4.81 (70)                          |                            |
| 2,4-Dimethylphenol                      | 5.06 (30)                          | 1.48 (20, B), 1.98 (60, B) |
| 2,5-Dimethylphenol                      | 5.36 (65)                          | 1.43 (20, B), 1.52 (60, B) |
| 2,6-Dimethylphenol                      | 4.90 (40)                          | 1.4                        |
| 3,4-Dimethylphenol                      | 9.02 (60)                          | 1.77 (20, B)               |
| 3,5-Dimethylphenol                      | 9.06 (50)                          | 1.76 (20, B)               |
| Dimethyl <i>o</i> -phthalate            | 8.66 (20), 8.25 (25), 8.11 (45)    | 2.8 (25, B)                |
| 2,2-Dimethylpropanal                    | 9.051 (20)                         | 2.66                       |
| <i>N,N</i> -Dimethylpropanamide         | 34.6 (20)                          |                            |
| 2,2-Dimethylpropanamide                 | 20.13 (25)                         |                            |
| 2,2-Dimethylpropane                     | 1.769 (23), 1.678 (98)             | 0                          |
| 2,2-Dimethylpropane nitrile             | 21.1 (20)                          | 3.95                       |
| <i>N,N</i> -Dimethylpropanamide         | 33.1                               |                            |
| 2,2-Dimethyl-1-propanol                 | 8.35 (60)                          |                            |
| 2,5-Dimethylpyrazine                    | 2.436 (20)                         | 0                          |
| 2,6-Dimethylpyrazine                    | 2.653 (35)                         |                            |
| 2,4-Dimethylpyridine                    | 9.60 (20)                          | 2.3                        |
| 2,6-Dimethylpyridine                    | 7.33 (20)                          | 1.7                        |
| 2,6-Dimethylpyridine-1-oxide            | 46.11 (25)                         |                            |
| 2,3-Dimethylquinoxaline                 | 2.3 (25)                           | 0                          |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                 | Dielectric constant, $\epsilon$ | Dipole moment, D            |
|-------------------------------------------|---------------------------------|-----------------------------|
| Dimethyl succinate                        | 7.19 (20)                       | 2.09 (20, B)                |
| Dimethyl sulfate                          | 55.0 (25)                       | 4.31 (25, D)                |
| Dimethyl sulfide                          | 6.70 (21)                       | 1.554                       |
| Dimethyl sulfite                          | 22.5 (23)                       | 2.93 (20, B)                |
| Dimethyl sulfone                          | 47.39 (110)                     |                             |
| Dimethyl sulfoxide                        | 47.24 (20), 41.9 (55)           | 3.96 (25, B)                |
| <i>cis</i> -2,5-Dimethyltetrahydrofuran   | 5.03 (23)                       |                             |
| <i>N,N</i> -Dimethylthioformamide         | 47.5 (25)                       |                             |
| <i>N,N</i> -Dimethyl- <i>o</i> -toluidine | 3.4 (20)                        | 0.88 (25, B)                |
| <i>N,N</i> -Dimethyl- <i>p</i> -toluidine | 3.9(20)                         | 1.29 (25, B)                |
| <i>m</i> -Dinitrobenzene                  | 22.9 (92)                       |                             |
| 2,2-Dinitropropane                        | 42.4 (52)                       |                             |
| Dinonyl hexanedioate                      |                                 | 2.53 (25, B)                |
| Dinonyl <i>o</i> -phthalate               | 4.65 (35), 4.52 (45)            |                             |
| Dioctyl decanedioate                      | 4.0 (27)                        |                             |
| Dioctyl <i>o</i> -phthalate               | 5.1 (25)                        | 3.06 (25, C)                |
| 1,4-Dioxane                               | 2.219 (20), 2.21 (25)           | 0                           |
| 1,3-Dioxolane                             |                                 | 1.19                        |
| 1,3-Dioxolan-2-one                        | 89.78 (40)                      |                             |
| Dipentene                                 | 2.38 (25)                       |                             |
| Dipentyl ether                            | 2.80 (25)                       | 0.98 (20, lq), 1.24 (25, B) |
| Dipentyl <i>o</i> -phthalate              | 5.79 (35), 5.62 (45)            | 2.71 (20, lq)               |
| Dipentyl sulfide                          | 3.83 (25)                       | 1.59 (25, B)                |
| Dipentylamine                             | 3.3 (52)                        | 1.31 (20, C), 1.01 (25, B)  |
| 1,2-Diphenylethane                        | 2.4 (110)                       | 0 (110, lq), 0.45 (25, B)   |
| Diphenyl ether                            | 3.73 (10), 3.63 (30)            | 1.3                         |
| Diphenylmethane                           | 2.7 (18), 2.57 (26)             | 0.26 (30, lq), 0.3 (25, B)  |
| Dipropylamine                             | 2.923 (20)                      | 1.01 (20, lq), 1.03 (20, B) |
| Dipropyl ether                            | 3.38 (24)                       | 1.21                        |
| <i>N,N</i> -Dipropylformamide             | 23.5 (20)                       |                             |
| Dipropyl sulfone                          | 32.62 (30)                      |                             |
| Dipropyl sulfoxide                        | 30.37 (30)                      |                             |
| Divinyl ether                             | 3.94 (15)                       | 0.78                        |
| Dodecamethylcyclohexasiloxane             | 2.6 (20)                        |                             |
| Dodecamethylpentasiloxane                 | 2.5 (20)                        |                             |
| Dodecane                                  | 2.05 (– 10), 2.01 (20)          | 0                           |
| 1-Dodecanol                               | 5.15 (20), 6.5 (25)             | 1.52 (20, B)                |
| 1-Dodecene                                | 2.15 (20)                       | 0                           |
| 6-Dodecyne                                | 2.17 (25)                       |                             |
| 1,2-Epoxybutane                           |                                 | 2.01 (20, B)                |
| Erythritol                                | 28 (128)                        |                             |
| Ethane                                    | 1.936 (– 178), 1.0015 (0)       | 0                           |
| 1,2-Ethanediamine                         | 16.8 (18), 13.82 (20)           | 1.96                        |
| 1,2-Ethandiol                             | 41.4 (20), 37.7 (25)            | 2.28                        |
| 1,2-Ethandiol diacetate                   | 7.7 (17)                        | 2.34 (30, B)                |
| 1,2-Ethandiol dinitrate                   | 28.26 (20)                      |                             |
| 1,2-Ethandiol monoacetate                 | 12.95 (30)                      |                             |
| 1,2-Ethanedithiol                         | 7.26 (20)                       |                             |
| Ethanesulfonyl chloride                   |                                 | 3.89 (25, B)                |
| Ethanethiol                               | 6.9 (15), 6.667 (25)            | 1.58                        |
| Ethanol                                   | 25.3 (20), 20.21 (55)           | 1.69                        |
| Ethanolamine                              | 31.94 (20)                      |                             |



**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                             | Dielectric constant, $\epsilon$ | Dipole moment, D                                                   |
|---------------------------------------|---------------------------------|--------------------------------------------------------------------|
| Ethoxyacetylene                       | 8.05 (25)                       |                                                                    |
| 4-Ethoxyaniline                       | 7.43 (25)                       |                                                                    |
| Ethoxybenzene (phenetol)              | 4.216 (20)                      | 1.45                                                               |
| 2-Ethoxyethanol                       | 13.38 (25)                      | 2.24 (30, B)                                                       |
| 2-Ethoxyethyl acetate                 | 7.567 (30)                      | 2.25 (30, B)                                                       |
| 1-Ethoxy-2-methylbutane               | 3.96 (20)                       |                                                                    |
| 1-Ethoxynaphthalene                   | 3.3 (19)                        |                                                                    |
| 1-Ethoxypentane                       | 3.6 (23)                        |                                                                    |
| $\alpha$ -Ethoxytoluene               | 3.9 (20)                        |                                                                    |
| Ethoxytrimethylsilane                 | 3.013 (25)                      |                                                                    |
| <i>N</i> -Ethylacetamide              | 135.0 (20)                      |                                                                    |
| Ethyl acetate                         | 6.081 (20), 5.30 (77)           | 1.78                                                               |
| Ethyl acetoacetate                    | 14.0 (20)                       | 3.22 (18, B, keto form)<br>2.04 (–80, CS <sub>2</sub> , enol form) |
| Ethyl acrylate                        | 6.05 (30)                       | 2.0                                                                |
| Ethylamine                            | 8.7 (0), 6.94 (10)              | 1.22                                                               |
| <i>N</i> -Ethylaniline                | 5.87 (20)                       |                                                                    |
| 4-Ethylaniline                        | 4.84 (25)                       |                                                                    |
| Ethylbenzene                          | 2.446 (20)                      | 0.59                                                               |
| Ethyl benzoate                        | 6.20 (20)                       | 2.00                                                               |
| Ethyl 2-bromoacetate                  | 8.75 (30)                       |                                                                    |
| Ethyl $\alpha$ -bromobutanoate        | 8 (20)                          | 2.40 (25, B)                                                       |
| Ethyl 2-bromo-2-methylpropanoate      | 8.55 (30)                       |                                                                    |
| Ethyl 2-bromopropanoate               | 9.4 (20), 8.57 (30)             |                                                                    |
| <i>N</i> -Ethylbutanamide             | 107.0 (25)                      |                                                                    |
| Ethyl butanoate                       | 5.18 (28)                       | 1.74 (22, B)                                                       |
| 2-Ethylbutanoic acid                  | 2.72 (23)                       |                                                                    |
| 2-Ethyl-1-butanol                     | 6.19 (90)                       |                                                                    |
| Ethyl <i>tert</i> -butyl ether        | 7.07 (25)                       |                                                                    |
| Ethyl carbamate                       | 14.2 (50), 14.14 (55)           | 2.59 (30, D)                                                       |
| Ethyl chloroacetate                   | 11.4 (21)                       | 2.65 (25, B)                                                       |
| Ethyl chlorocarbonate                 | 9.736 (36)                      |                                                                    |
| Ethyl <i>cis</i> -3-chlorocrotonate   | 7.67 (76)                       |                                                                    |
| Ethyl <i>trans</i> -3-chlorocrotonate | 4.70 (54)                       |                                                                    |
| Ethyl chloroformate                   | 11 (20)                         | 2.56 (35, B)                                                       |
| Ethyl 2-chloropropanoate              | 11.95 (30)                      |                                                                    |
| Ethyl 3-chloropropanoate              | 10.19 (30)                      |                                                                    |
| Ethyl <i>trans</i> -cinnamate         | 6.1 (18), 5.83 (20)             | 1.86 (20, B)                                                       |
| Ethyl crotonate                       | 5.4 (20)                        | 1.95 (24, B)                                                       |
| Ethyl cyanoacetate                    | 31.62 (–10), 26.9 (20)          | 2.2                                                                |
| Ethylcyclobutane                      | 1.965 (20)                      |                                                                    |
| Ethylcyclohexane                      | 2.054 (20)                      | 0                                                                  |
| Ethylcyclopropane                     | 1.933 (20)                      |                                                                    |
| Ethyl dichloroacetate                 | 12 (2), 10 (22)                 | 2.63 (25, B)                                                       |
| Ethyl dodecanoate                     | 3.4 (20), 2.7 (143)             | 1.3 (20, lq)                                                       |
| Ethylene                              | 1.001 44 (0, g), 1.483 (–3)     | 0                                                                  |
| Ethylene carbonate                    | 89.78 (40), 69.4 (91)           | 4.87 (25, B)                                                       |
| Ethylenediamine                       | 13.82 (20)                      | 1.98                                                               |
| Ethylene dinitrate                    | 28.3 (20)                       | 3.58 (25, B)                                                       |
| 2,2'-(Ethylenedioxy)diethanol         | 23.69 (20)                      | 5.58 (lq)                                                          |
| Ethylene glycol                       | 41.4 (20), 37.7 (25)            | 2.28                                                               |
| Ethylene glycol diacetate             | 7.7 (17)                        |                                                                    |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                         | Dielectric constant, $\epsilon$ | Dipole moment, D |
|-----------------------------------|---------------------------------|------------------|
| Ethyleneimine                     | 18.3 (25)                       | 1.90             |
| Ethylene oxide                    | 14 (–1), 12.42 (20)             | 1.89             |
| Ethylene sulfite                  | 39.6 (25)                       |                  |
| <i>N</i> -Ethylformamide          | 102.7 (25)                      |                  |
| Ethyl formate                     | 8.57 (15), 7.16 (25)            | 1.94             |
| Ethyl fumarate                    | 6.5 (23)                        |                  |
| Ethyl furan-2-carboxylate         | 9.02 (20)                       |                  |
| Ethylhexadecanoate                | 3.2 (20), 2.71 (104)            | 1.2 (lq)         |
| 3-Ethylhexane                     | 1.96 (20)                       | 0                |
| 2-Ethyl-1,2-hexanediol            | 18.73 (20)                      |                  |
| Ethyl hexanoate                   | 4.45 (20)                       | 1.80 (20, B)     |
| 2-Ethyl-1-hexanol                 | 7.58 (25), 4.41 (90)            | 1.74 (25, B)     |
| 2-Ethylhexyl acetate              |                                 | 1.8              |
| Ethyl 2-iodopropanoate            | 8.6 (20)                        |                  |
| Ethyl isocyanate                  | 19.7 (20)                       |                  |
| Ethyl isopentyl ether             | 3.96 (20)                       |                  |
| Ethyl isothiocyanate              | 19.6 (20)                       | 3.67 (20, B)     |
| Ethyl lactate                     | 15.4 (30)                       | 2.4 (20, B)      |
| Ethyl maleate                     | 8.6 (23)                        |                  |
| Ethyl methacrylate                | 5.68 (30)                       |                  |
| Ethyl 3-methylbutanoate           | 4.71 (20)                       |                  |
| Ethyl- <i>N</i> -methyl carbamate | 21.10 (25)                      |                  |
| Ethyl methyl carbonate            | 2.985 (20)                      |                  |
| Ethyl methyl ether                |                                 | 1.17             |
| 3-Ethyl-2-methylpentane           | 1.99 (18)                       | 0                |
| Ethyl nitrate                     | 19.7 (20)                       | 2.93 (20, B)     |
| Ethyl 9-octadecanoate             | 3.2 (25)                        | 1.83 (20, lq)    |
| 3-Ethylloxazolidine-2-one         | 66.8 (25)                       |                  |
| 4-Ethylloxazolidine-2-one         | 42.6 (25)                       |                  |
| Ethyl 4-oxopentanoate             | 12 (21)                         |                  |
| 3-Ethylpentane                    | 1.942 (20)                      | 0                |
| Ethyl pentanoate                  | 4.71 (18)                       | 1.76 (28, B)     |
| 3-Ethyl-3-pentanol                | 3.158 (20)                      |                  |
| Ethyl pentyl ether                | 3.6 (23)                        | 1.2 (20, B)      |
| Ethyl phenylacetate               | 5.3 (21)                        | 1.82 (30)        |
| Ethyl phenyl sulfide              |                                 | 4.08 (25, B)     |
| <i>N</i> -Ethyl propanamide       | 126.8 (25)                      |                  |
| Ethyl propanoate                  | 5.76 (20)                       | 1.75 (22, B)     |
| Ethyl propyl ether                |                                 | 1.16 (25, B)     |
| 2-Ethylpyridine                   | 8.33 (20)                       |                  |
| 4-Ethylpyridine                   | 10.98 (20)                      |                  |
| Ethyl salicylate                  | 7.99 (30)                       | 2.85 (25, B)     |
| Ethyl stearate                    | 2.98 (40), 2.69 (100)           | 1.65 (40, lq)    |
| Ethyl thiocyanate                 | 29.3 (21)                       | 3.33 (20, B)     |
| <i>p</i> -Ethyltoluene            | 2.24 (25)                       | 0                |
| Ethyl trichloroacetate            | 8.428 (20)                      | 2.56 (25, B)     |
| Ethyltrimethylsilazine            | 2.275 (30)                      |                  |
| Ethyl vinyl ether                 |                                 | 1.26 (20, B)     |
| Fluorobenzene                     | 5.465 (20), 5.42 (25), 4.7 (60) | 1.60             |
| 4-Fluorobenzene sulfonylchloride  | 12.65 (40)                      |                  |
| 2-Fluoroiodobenzene               | 8.22 (25)                       |                  |
| 3-Fluoroiodobenzene               | 4.62 (25)                       |                  |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                           | Dielectric constant, $\epsilon$ | Dipole moment, D            |
|-------------------------------------|---------------------------------|-----------------------------|
| 4-Fluoroiodobenzene                 | 3.12 (25)                       |                             |
| Fluoromethane                       | 51.0 (– 142)                    | 1.858                       |
| 2-Fluoro-2-methylbutane             | 5.89 (20)                       | 1.92 (25, B)                |
| 1-Fluoropentane                     | 3.93 (20)                       | 1.85 (25, B)                |
| <i>o</i> -Fluorotoluene             | 4.23 (25), 4.22 (30), 3.9 (60)  | 1.37                        |
| <i>m</i> -Fluorotoluene             | 5.41 (25), 4.9 (60)             | 1.82                        |
| <i>p</i> -Fluorotoluene             | 5.88 (25), 5.86 (30), 5.3 (60)  | 2.00                        |
| Formamide                           | 111.0 (20), 103.5 (40)          | 3.73                        |
| Formanilide                         |                                 | 3.37 (25, C)                |
| Formic acid                         | 58.5 (15), 57.0 (21), 51.1 (25) | 1.41                        |
| 2-Furaldehyde                       | 42.1 (20), 34.9 (50)            | 3.63 (25, B)                |
| Furan                               | 2.88 (4)                        | 0.66                        |
| 2-Furfuryl acetate                  | 5.85 (20)                       |                             |
| Furfuryl alcohol                    | 16.85 (25)                      | 1.92 (25, lq)               |
| Glycerol                            | 46.5 (20), 42.5 (25)            | 2.68 (25, D)                |
| Glycerol tris(acetate)              | 7.2 (20)                        | 2.73 (25, B)                |
| Glycerol tris(nitrate)              | 19.25 (20)                      | 3.38 (25, B)                |
| Glycerol tris(oleate)               | 3.2 (26)                        | 3.11 (23, B)                |
| Glycerol tris(palmitate)            | 2.9 (65)                        | 2.80 (23, B)                |
| Glycerol tris(sterate)              | 2.8 (70)                        | 2.86 (23, B)                |
| 1,6-Heptadiene                      | 2.161 (20)                      |                             |
| Heptacosafuorotributylamine         | 2.15 (20)                       |                             |
| 2,2,3,3,4,4,4-Heptafluoro-1-butanol | 14.4 (25)                       |                             |
| Heptanal                            | 9.1 (20)                        | 2.26 (40, lq), 2.58 (22, B) |
| Heptane                             | 1.921 (20), 1.85 (70)           | 0                           |
| 1-Heptanethiol                      | 4.194 (20)                      |                             |
| Heptanoic acid                      | 3.04 (15), 2.6 (71)             |                             |
| 1-Heptanol                          | 11.75 (20)                      | 1.73 (20, B)                |
| ( $\pm$ )-2-Heptanol                | 9.72 (21)                       | 1.73 (20, B)                |
| ( $\pm$ )-3-Heptanol                | 7.07 (23)                       | 1.73 (20, B)                |
| 4-Heptanol                          | 6.18 (23)                       | 1.72 (20, B)                |
| 2-Heptanone                         | 11.95 (20), 8.27 (100)          | 2.61 (22, B)                |
| 3-Heptanone                         | 12.7 (20)                       | 2.81 (22, B)                |
| 4-Heptanone                         | 12.60 (20), 9.46 (80)           | 2.74 (20, B)                |
| 1-Heptene                           | 2.09 (20)                       | 0                           |
| Heptylamine                         | 3.81 (20)                       |                             |
| Hexachloroacetone                   | 3.93 (19)                       |                             |
| Hexachloro-1,3-butadiene            | 2.55 (20)                       |                             |
| Hexadecamethylcyclooctasiloxane     | 2.7 (20)                        |                             |
| Hexadecane                          | 2.046 (30)                      | 0                           |
| 1-Hexadecanol                       | 3.8 (50)                        | 1.67 (25, B)                |
| 1,5-Hexadiene                       | 2.125 (26)                      |                             |
| 2,4-Hexadiene                       | 2.207 (25)                      | 0.31 (25, B)                |
| <i>cis,cis</i> -2,4-Hexadiene       | 2.163 (24)                      |                             |
| <i>trans,trans</i> -2,4-Hexadiene   | 2.123 (24)                      |                             |
| Hexafluoroacetone                   | 2.104 (– 71)                    |                             |
| Hexafluorobenzene                   | 2.029 (25)                      | 0                           |
| 1,1,1,3,3,3-Hexafluoro-2-propanol   | 16.70 (20)                      |                             |
| Hexamethyldisiloxane                | 2.2 (20)                        | 0.37 (25, lq)               |
| Hexamethylphosphorotriamide         | 31.3 (20)                       | 5.5, 4.31 (25, lq)          |
| Hexane                              | 1.904 (15), 1.890 (20)          | 0                           |
| Hexanedinitrile                     | 32.45 (25)                      | 3.8 (25, B)                 |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                           | Dielectric constant, $\epsilon$ | Dipole moment, D            |
|-------------------------------------|---------------------------------|-----------------------------|
| Hexanenitrile                       | 17.26 (25)                      |                             |
| 1-Hexanethiol                       | 4.436 (20)                      |                             |
| 1,2,6-Hexanetriol                   | 31.5 (12)                       |                             |
| Hexanoic acid                       | 2.600 (25)                      | 1.13 (25, lq)               |
| 1-Hexanol                           | 13.03 (20), 8.5 (75)            | 1.55 (20, B)                |
| ( $\pm$ )-2-Hexanol                 | 11.06 (25)                      |                             |
| 3-Hexanol                           | 9.66 (25)                       |                             |
| 2-Hexanone                          | 14.6 (15), 14.56 (20)           | 2.68 (22, B)                |
| 1-Hexene                            | 2.051 (20)                      | 0                           |
| <i>cis</i> -2-Hexene                |                                 | 0                           |
| <i>trans</i> -2-Hexene              | 1.978 (22)                      | 0                           |
| <i>cis</i> -3-Hexene                | 2.069 (23)                      | 0                           |
| <i>trans</i> -3-Hexene              | 1.954 (20)                      | 0                           |
| Hexyl acetate                       | 4.42 (20)                       |                             |
| Hexylamine                          | 4.08 (20)                       |                             |
| 1-Hexyne                            | 2.621 (23)                      | 0.83                        |
| 2-Hydroxyacetophenone               | 21.33 (25)                      |                             |
| 2-Hydroxybutanoic acid              | 37.7 (23)                       |                             |
| 3-Hydroxybutanoic acid              | 31.5 (23)                       |                             |
| <i>N</i> -(2-Hydroxyethyl)acetamide | 96.6 (25)                       |                             |
| 4-Hydroxy-4-methyl-2-pentanone      | 18.2 (25)                       | 3.24 (20, B)                |
| 3-Hydroxypropanoic acid             | 30.0 (23)                       |                             |
| Iodobenzene                         | 4.59 (20)                       | 1.70                        |
| 1-Iodobutane                        | 6.27 (20), 4.52 (130)           | 2.10                        |
| 2-Iodobutane                        | 7.873 (20)                      | 2.12                        |
| 1-Iodododecane                      | 3.9 (20)                        | 1.87 (20, C)                |
| Iodoethane                          | 10.2 (–50), 7.82 (20)           | 1.91                        |
| 1-Iodoheptane                       | 4.92 (22)                       | 1.86 (22, B)                |
| 3-Iodoheptane                       | 6.39 (22)                       | 1.95 (22, B)                |
| 1-Iodohexadecane                    | 3.5 (20)                        |                             |
| 1-Iodohexane                        | 5.37 (20)                       | 1.94 (20, C)                |
| Iodomethane                         | 6.97 (20)                       | 1.62                        |
| 1-Iodo-3-methylbutane               | 5.6 (19)                        | 1.85 (20, B)                |
| 2-Iodo-2-methylbutane               | 8.19 (20)                       | 2.20 (20, B)                |
| 1-Iodo-2-methylpropane              | 6.47 (20)                       | 1.89 (20, B)                |
| 2-Iodo-2-methylpropane              | 6.65 (10)                       |                             |
| 1-Iodooctane                        | 4.6 (25)                        | 1.80 (25, lq), 1.90 (20, C) |
| 2-Iodooctane                        | 5.8 (20)                        | 2.07 (20, C)                |
| 1-Iodopentane                       | 5.78 (20)                       | 1.90 (20, B)                |
| 3-Iodopentane                       | 7.432 (20)                      |                             |
| 1-Iodopropane                       | 7.07 (20)                       | 2.03                        |
| 2-Iodopropane                       | 8.19 (25)                       | 2.01 (20, B)                |
| 3-Iodopropene                       | 6.1 (19)                        |                             |
| <i>p</i> -Iodotoluene               | 4.4 (35)                        | 1.72 (22, B)                |
| $\alpha$ -Ionone                    | 11 (18)                         |                             |
| $\beta$ -Ionone                     | 12 (20)                         |                             |
| Iron pentacarbonyl                  | 2.602 (20)                      |                             |
| Isobutanenitrile                    | 20.4 (24)                       | 3.61 (25, B)                |
| Isobutene                           | 2.1225 (15)                     | 0.503                       |
| <i>N</i> -Isobutylacetamide         | 111.0 (20)                      |                             |
| Isobutyl acetate                    | 5.068 (20)                      | 1.87 (22, B)                |
| Isobutylamine                       | 4.43 (21)                       | 1.27 (25, B)                |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                           | Dielectric constant, $\epsilon$  | Dipole moment, D            |
|-------------------------------------|----------------------------------|-----------------------------|
| Isobutylbenzene                     | 2.319 (20), 2.298 (30)           | 0.31 (20, lq)               |
| Isobutyl butanoate                  | 4.1 (20)                         | 1.9                         |
| Isobutyl chlorocarbonate            | 9.1 (20)                         |                             |
| Isobutyl formate                    | 6.41 (20)                        | 1.89 (20, B)                |
| Isobutyl isocyanate                 | 11.64 (20)                       |                             |
| Isobutyl nitrate                    | 2.7 (20)                         |                             |
| Isobutyl pentanoate                 | 3.8 (19)                         |                             |
| Isobutylsilane                      | 2.497 (20)                       |                             |
| Isobutyl trichloroacetate           | 7.667 (20)                       |                             |
| Isobutyl vinyl ether                | 3.34 (20)                        |                             |
| Isobutyronitrile                    | 20.4 (24)                        | 3.61 (25, B)                |
| Isopentyl acetate                   | 4.72 (20), 4.63 (30)             | 1.84 (22, B), 1.76 (30, lq) |
| Isopentyl butanoate                 | 4.0 (20)                         |                             |
| Isopentyl pentanoate                | 3.6 (19)                         | 1.8 (28, B)                 |
| Isopentyl propanoate                | 4.2 (20)                         |                             |
| Isopropyl acetate                   |                                  | 1.86 (22, B)                |
| Isopropylamine                      | 5.627 (20)                       | 1.19                        |
| Isopropylbenzene                    | 2.38 (20)                        | 0.79                        |
| Isopropyl carborane                 | 45.0 (20)                        |                             |
| <i>N</i> -Isopropylformamide        | 65.7 (25)                        |                             |
| 1-Isopropyl-4-methylbenzene         | 2.24 (20)                        | 0                           |
| Isopropyl nitrite                   | 13.92 (– 13)                     |                             |
| Isoquinoline                        | 11.0 (25)                        | 2.73                        |
| Lactic acid                         | 22 (17)                          |                             |
| Lactonitrile                        | 38 (20)                          |                             |
| <b>D</b> -Limonene                  | 2.4 (20), 2.37 (25)              | 1.57 (25, B)                |
| ( $\pm$ )-Limonene                  | 2.3 (20)                         | 0.63 (25, B)                |
| Maleic anhydride                    | 52.75 (53)                       |                             |
| ( $\pm$ )-Mandelonitrile            | 17.8 (23)                        |                             |
| <b>D</b> -Mannitol                  | 24.6 (170)                       |                             |
| Menthol                             |                                  | 1.55 (20, B)                |
| Methacrylic acid                    |                                  | 1.65                        |
| Methacrylonitrile                   |                                  | 3.69                        |
| Methane                             | 1.676 (– 182), 1.000 94 (0)      | 0                           |
| Methanesulfonyl chloride            | 34.0 (20)                        |                             |
| Methanethiol                        |                                  | 1.52 (g)                    |
| Methanol                            | 41.8 (– 20), 33.0 (20)           | 1.70                        |
| 2-Methoxyaniline                    | 5.230 (30)                       |                             |
| 3-Methoxyaniline                    | 8.76 (25)                        |                             |
| 4-Methoxyaniline                    | 7.85 (60)                        |                             |
| <i>o</i> -Methoxybenzaldehyde       |                                  | 4.34 (20, B)                |
| <i>p</i> -Methoxybenzaldehyde       | 22.3 (22), 22.0 (30), 10.4 (248) | 3.26 (35, B)                |
| Methoxybenzene                      | 4.30 (21), 3.9 (70)              | 1.38                        |
| 2-Methoxyethanol                    | 17.2 (25), 16.0 (30)             | 2.36                        |
| <i>N</i> -(2-Methoxyethyl)acetamide | 80.7 (25)                        |                             |
| 2-Methoxyethyl acetate              | 8.25 (20)                        | 2.13 (30, B)                |
| 1-Methoxy-2-nitrobenzene            | 45.75 (20)                       | 4.83                        |
| <i>o</i> -Methoxyphenol             | 11.95 (25)                       |                             |
| <i>m</i> -Methoxyphenol             | 11.59 (25)                       |                             |
| <i>p</i> -Methoxyphenol             | 11.05 (60)                       |                             |
| 2-Methoxy-4-(2-propenyl)phenol      |                                  | 2.46 (25, B)                |
| <i>o</i> -Methoxytoluene            | 3.5 (20)                         |                             |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                          | Dielectric constant, $\epsilon$     | Dipole moment, D            |
|------------------------------------|-------------------------------------|-----------------------------|
| <i>m</i> -Methoxytoluene           | 3.5 (20)                            |                             |
| <i>p</i> -Methoxytoluene           | 4.0 (20)                            |                             |
| Methoxytrimethylsilane             | 3.248 (25)                          |                             |
| <i>N</i> -Methylacetamide          | 178.9 (30), 138.6 (60)              | 4.39 (20, D)                |
| Methyl acetate                     | 7.07 (15), 7.03 (20), 6.68 (25)     | 1.72                        |
| Methyl acrylate                    | 7.03 (30)                           | 1.77 (25, B)                |
| Methylamine                        | 16.7 (− 58), 11.4 (− 10), 10.0 (18) | 1.31                        |
| Methyl 2-aminobenzoate             | 21.9 (25)                           |                             |
| <i>N</i> -Methylaniline            | 5.96 (20)                           | 1.67 (25, B)                |
| 2-Methylaniline                    | 6.138 (25)                          |                             |
| 3-Methylaniline                    | 5.816 (25)                          |                             |
| 4-Methylaniline                    | 5.058 (25)                          |                             |
| <i>N</i> -Methylbenzenesulfonamide | 67.1 (30)                           |                             |
| Methyl benzoate                    | 6.64 (30)                           | 1.86 (25, B)                |
| 2-Methyl-1,2-butadiene             | 2.1 (25)                            | 0.15                        |
| 2-Methyl-1,3-butadiene             | 2.098 (20)                          | 0.25                        |
| 2-Methylbutane                     | 1.871 (0), 1.845 (20)               | 0.13                        |
| 2-Methyl-2-butanethiol             | 5.083 (20)                          |                             |
| Methyl butanoate                   | 5.6 (20), 5.48 (29)                 | 1.72 (22, B)                |
| 3-Methylbutanoic acid              | 2.64 (20)                           | 0.63 (25)                   |
| 2-Methyl-1-butanol                 | 15.63 (25)                          | 1.9                         |
| 2-Methyl-2-butanol                 | 5.78 (25)                           | 1.72 (20, B)                |
| 3-Methyl-1-butanol                 | 15.63 (20), 14.7 (25), 5.82 (130)   | 1.82 (25, B)                |
| 3-Methyl-2-butanol                 | 12.1 (25)                           |                             |
| 3-Methyl-2-butanone                | 10.37 (20)                          |                             |
| 2-Methyl-1-butene                  | 2.180 (20)                          | 0.52 (20, lq)               |
| 2-Methyl-2-butene                  | 1.979 (23)                          | 0.11 (25, lq), 0.34 (25, B) |
| 3-Methyl-1-butene                  | 1.0028 (100, g)                     | 0.320                       |
| 2-Methyl-1-butene-2-one            | 10.39 (30)                          |                             |
| 2-Methylbutyl acetate              | 4.63 (30)                           | 1.82 (22)                   |
| 3-Methylbutyl 3-methylbutanoate    | 4.39 (15)                           |                             |
| 3-Methylbutyronitrile              | 18 (220)                            | 3.62 (25, C)                |
| Methyl carbamate                   | 18.48 (55)                          |                             |
| Methyl chloroacetate               | 12.0 (20)                           |                             |
| <i>N</i> -Methyl-2-chloroacetamide | 92.3 (50)                           |                             |
| Methyl 4-chlorobutanoate           | 9.51 (30)                           |                             |
| Methyl crotonate                   | 6.664 (20)                          |                             |
| Methyl cyanoacetate                | 29.3 (20), 19.23 (50), 17.57 (65)   |                             |
| Methylcyclohexane                  | 2.024 (20)                          | 0                           |
| 2-Methylcyclohexanol               |                                     | 1.95 (25, B)                |
| <i>cis</i> -3-Methylcyclohexanol   | 16.05 (20)                          | 1.91                        |
| <i>trans</i> -3-Methylcyclohexanol | 8.05 (20)                           | 1.75                        |
| 4-Methylcyclohexanol               |                                     | 1.9 (25, B)                 |
| 2-Methylcyclohexanone              | 16 (− 15), 14.0 (20)                | 2.98 (25, B)                |
| 3-Methylcyclohexanone              | 18 (− 80), 12.4 (20)                | 3.06 (25, B)                |
| 4-Methylcyclohexanone              | 15 (− 41), 12.35 (20)               | 3.07 (25, B)                |
| Methylcyclopentane                 | 1.985 (20)                          | 0                           |
| 1-Methylcyclopentanol              | 7.11 (37)                           |                             |
| Methyl decanoate                   |                                     | 1.65 (20, Hx)               |
| Methyl dodecanoate                 |                                     | 1.70 (20, Hx)               |
| <i>N</i> -Methylformamide          | 200.1 (15), 189.0 (20), 182.4 (25)  | 3.83                        |
| Methyl formate                     | 9.20 (15), 8.5 (20)                 | 1.77                        |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                       | Dielectric constant, $\epsilon$ | Dipole moment, D |
|---------------------------------|---------------------------------|------------------|
| 2-Methylfuran                   | 2.76 (20)                       | 0.65             |
| Methyl furan-2-carboxylate      | 11.01 (20)                      |                  |
| (mono)Methyl glutarate          | 8.37 (20)                       |                  |
| 2-Methylheptane                 | 1.95 (20)                       | 0                |
| 2-Methyl-2-heptanol             | 3.38 (– 7), 2.46 (25)           |                  |
| 2-Methyl-3-heptanol             | 3.37 (20), 3.75 (60)            | 1.63 (20, B)     |
| 2-Methyl-4-heptanol             | 3.30 (20), 3.65 (60)            |                  |
| 3-Methyl-3-heptanol             | 3.74 (20), 2.89 (60)            |                  |
| 3-Methyl-4-heptanol             | 9.1 (– 20), 7.4 (20)            |                  |
| 4-Methyl-3-heptanol             | 5.25 (20), 4.62 (55)            |                  |
| 4-Methyl-4-heptanol             | 2.87 (20), 3.27 (60)            |                  |
| 2-Methylhexane                  | 1.922 (20)                      | 0                |
| 3-Methylhexane                  | 1.920 (20)                      | 0                |
| Methyl hexanoate                | 4.615 (20)                      | 1.70 (20, Hx)    |
| 2-Methyl-2-hexanol              | 3.257 (24)                      |                  |
| 3-Methyl-2-hexanol              | 4.990 (24)                      |                  |
| 3-Methyl-3-hexanol              | 3.248 (25)                      |                  |
| 5-Methyl-2-hexanone             | 13.53 (20)                      |                  |
| Methyl isobutanoate             |                                 | 1.98 (20, B)     |
| Methylisocyanate                | 21.75 (16)                      | 2.8              |
| Methyl methacrylate             | 6.32 (30)                       | 1.68 (25, B)     |
| N-Methyl methanesulfonamide     | 104.4 (25)                      |                  |
| Methyl o-methoxybenzene         | 7.7 (21)                        |                  |
| Methyl p-methoxybenzoate        | 4.3 (33)                        |                  |
| N-Methyl-2-methylbutanamide     | 123.0 (34)                      |                  |
| N-Methyl-3-methylbutanamide     | 114.0 (26)                      |                  |
| Methyl 3-(methylthio)propanoate | 8.66 (30)                       |                  |
| 1-Methylnaphthalene             | 2.92 (20)                       | 0                |
| Methyl nitrate                  | 23.9 (20)                       |                  |
| Methyl nitrite                  | 20.77 (– 73)                    |                  |
| Methyl o-nitrobenzoate          | 28 (25)                         | 3.67 (30, B)     |
| 2-Methyloctane                  | 1.97 (20)                       | 0                |
| 3-Methyloctane                  |                                 | 0                |
| 4-Methyloctane                  | 1.97 (20)                       | 0                |
| Methyl oleate                   | 3.211 (20)                      |                  |
| 2-Methyl-1,3-pentadiene         | 2.422 (25)                      |                  |
| 3-Methyl-1,3-pentadiene         | 2.426 (25)                      |                  |
| 4-Methyl-1,3-pentadiene         | 2.599 (20)                      |                  |
| N-Methylpentanamide             | 131.0 (13)                      |                  |
| 2-Methylpentane                 | 1.886 (20)                      | 0                |
| 3-Methylpentane                 | 1.886 (20)                      | 0                |
| 2-Methyl-2,4-pentanediol        | 23.4 (20)                       | 2.9              |
| 4-Methylpentanenitrile          | 17.5 (22)                       | 3.53 (25, B)     |
| Methyl pentanoate               | 4.992 (20)                      | 1.62 (22, B)     |
| 3-Methyl-1-pentanol             | 15.2 (25)                       |                  |
| 3-Methyl-3-pentanol             | 4.322 (20)                      |                  |
| 4-Methyl-2-pentanone            | 15.6 (0), 15.1 (20), 11.78 (40) |                  |
| 4-Methylpentenenitrile          | 17.5 (22)                       | 3.5              |
| 4-Methyl-3-penten-2-one         | 15.6 (0)                        | 2.8              |
| 1-Methyl-1-phenylhydrazine      | 7.3 (19)                        | 1.84 (15, B)     |
| Methyl phenyl sulfide           |                                 | 1.38 (20, B)     |
| Methyl phenyl sulfone           | 37.9 (100)                      |                  |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                | Dielectric constant, $\epsilon$   | Dipole moment, D |
|------------------------------------------|-----------------------------------|------------------|
| 2-Methylpropanal                         |                                   | 2.6              |
| <i>N</i> -Methylpropanamide              | 170.0 (20), 151 (40)              | 3.59             |
| 2-Methyl-1-propanamine                   | 4.43 (21)                         | 1.3              |
| 2-Methylpropane                          | 1.752 (25)                        | 0.132            |
| 2-Methylpropanenitrile                   | 24.42 (20)                        | 4.29             |
| 2-Methyl-1-propanethiol                  | 4.961 (25)                        |                  |
| 2-Methyl-2-propanethiol                  | 5.475 (20)                        | 1.66             |
| Methyl propanoate                        | 6.200 (20)                        | 1.70 (22, B)     |
| 2-Methylpropanoic acid                   | 2.58 (20)                         | 1.08 (25, lq)    |
| 2-Methylpropanoic anhydride              | 13.6 (19)                         |                  |
| 2-Methyl-1-propanol                      | 26 (– 34), 17.93 (20)             | 1.64             |
| 2-Methyl-2-propanol                      | 12.47 (25), 10.9 (30), 8.49 (50)  | 1.67 (22, B)     |
| 2-Methylpropene                          |                                   | 0.50             |
| 2-Methyl-2-propenenitrile                |                                   | 3.69             |
| 2-Methylpropenoic acid                   |                                   | 1.6              |
| 2-Methylpropyl acetate                   | 5.07 (20)                         | 1.87 (22, B)     |
| 2-Methyl-1-propylamine                   | 4.43 (21)                         | 1.27 (27)        |
| (2-Methylpropyl)benzene                  | 2.32 (20)                         | 0                |
| 2-Methylpropyl formate                   | 6.41 (20)                         | 1.88 (22)        |
| 2-Methylpyridine                         | 10.18 (20)                        | 1.85             |
| 3-Methylpyridine                         | 11.10 (30)                        | 2.41 (25, B)     |
| 4-Methylpyridine                         | 12.2 (20)                         | 2.70             |
| 2-Methylpyridine-1-oxide                 | 36.4 (50)                         |                  |
| 3-Methylpyridine-1-oxide                 | 28.26 (45)                        |                  |
| <i>N</i> -Methylpyrrolidine              | 32.2 (25)                         |                  |
| <i>N</i> -Methyl-2-pyrrolidinone         | 32.55 (20), 32.2 (25)             | 4.09 (30, B)     |
| Methyl salicylate                        | 9.41 (30), 8.80 (41)              | 2.47 (25, B)     |
| 3-Methyl sulfolane                       | 29.4 (25)                         |                  |
| Methyl tetradecanoate                    |                                   | 1.62 (25, B)     |
| 2-Methyltetrahydrofuran                  | 6.97 (25)                         |                  |
| Methyl tetrahydrothiophene-2-carboxylate | 7.30 (20)                         |                  |
| Methyl thiocyanate                       | 4.3 (19)                          | 3.34 (20, B)     |
| 2-Methylthiophene                        |                                   | 0.674            |
| 3-Methylthiophene                        |                                   | 0.95             |
| Methyl thiophene-2-carboxylate           | 8.81 (20)                         |                  |
| Methyl trifluoromethyl sulfone           | 32.0 (20)                         |                  |
| Morpholine                               | 7.42 (25)                         | 1.55             |
| $\beta$ -Myrcene                         | 2.3 (25)                          |                  |
| Naphthalene                              | 2.54 (90)                         | 0                |
| 1-Naphthonitrile                         | 16 (70)                           |                  |
| 2-Naphthonitrile                         | 17 (70)                           |                  |
| <i>o</i> -Nitroaniline                   | 47.3 (80), 34.5 (90)              | 4.28 (20, B)     |
| <i>m</i> -Nitroaniline                   | 35.6 (125)                        |                  |
| <i>p</i> -Nitroaniline                   | 78.5 (155), 56.3 (160)            | 6.3 (25, B)      |
| <i>o</i> -Nitroanisole                   | 45.75 (20)                        | 4.83             |
| <i>m</i> -Nitroanisole                   | 25.7 (45)                         |                  |
| <i>p</i> -Nitroanisole                   | 26.95 (65)                        |                  |
| Nitrobenzene                             | 35.6 (20), 34.82 (25), 24.9 (90)  | 4.22             |
| <i>m</i> -Nitrobenzyl alcohol            | 22 (20)                           |                  |
| 2-Nitrobiphenyl                          |                                   | 3.83 (20, B)     |
| Nitroethane                              | 29.11 (15), 28.06 (30), 27.4 (35) | 3.23             |



**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                                 | Dielectric constant, $\epsilon$   | Dipole moment, D            |
|-----------------------------------------------------------|-----------------------------------|-----------------------------|
| 2-Nitro-ethylbenzene                                      | 21.9 (0)                          |                             |
| Nitromethane                                              | 37.27 (20), 35.87 (30), 35.1 (35) | 3.46                        |
| 1-Nitro-2-methoxybenzene                                  |                                   | 4.83                        |
| <i>o</i> -Nitrophenol                                     | 16.50 (50)                        | 3.14 (25, B)                |
| <i>m</i> -Nitrophenol                                     | 35.45 (100)                       |                             |
| <i>p</i> -Nitrophenol                                     | 42.20 (120)                       |                             |
| 1-Nitropropane                                            | 24.70 (15), 23.24 (30), 22.7 (35) | 3.66                        |
| 2-Nitropropane                                            | 26.74 (15), 25.52 (30)            | 3.73                        |
| <i>N</i> -Nitrosodimethylamine                            | 53 (20)                           | 4.01 (20, B)                |
| <i>o</i> -Nitrotoluene                                    | 26.36 (20), 22.0 (58)             | 3.72 (20, B)                |
| <i>m</i> -Nitrotoluene                                    | 24.95 (30), 22 (58)               | 4.20 (20, B)                |
| <i>p</i> -Nitrotoluene                                    | 22.2 (58)                         | 4.47 (25, B)                |
| Nonane                                                    | 1.972 (20), 1.85 (110)            | 0                           |
| Nonanoic acid                                             | 2.48 (22)                         | 0.8                         |
| 1-Nonanol                                                 |                                   | 1.72 (20, B)                |
| 1-Nonene                                                  | 2.18 (20)                         | 0                           |
| ( <i>trans</i> , <i>trans</i> )-9,12-Octadecadienoic acid | 2.70 (70), 2.60 (120)             | 1.40 (18, Hx)               |
| Octamethylcyclotetrasiloxane                              | 2.4 (20)                          | 0.42 (25, lq), 0.67 (25, B) |
| Octamethyltrisiloxane                                     | 2.3 (20)                          | 0.64 (25, lq)               |
| Octane                                                    | 1.948 (20), 1.83 (110)            | 0                           |
| Octanenitrile                                             | 13.90 (20)                        |                             |
| Octanoic acid                                             | 2.85 (15), 2.45 (20)              | 1.15 (25, lq)               |
| 1-Octanol                                                 | 11.3 (10), 10.30 (20)             | 1.72 (20, B)                |
| 2-Octanol                                                 | 8.13 (20), 6.52 (40)              | 1.65 (20, B)                |
| 2-Octanone                                                | 9.51 (20), 7.42 (100)             | 2.72 (15, B)                |
| 1-Octene                                                  | 2.113 (20)                        | 0                           |
| <i>cis</i> -2-Octene                                      | 2.06 (25)                         | 0                           |
| <i>trans</i> -2-Octene                                    | 2.00 (25)                         | 0                           |
| Oleic acid                                                | 2.34 (20)                         | 1.2                         |
| Oxalyl chloride                                           | 3.470 (21)                        | 0.93 (20, B)                |
| Palmitic acid                                             | 2.3 (70)                          |                             |
| Paraldehyde                                               | 13.9 (25)                         | 1.43                        |
| Parathion                                                 |                                   | 4.98 (25, B)                |
| Pentachloroethane                                         | 3.73 (20), 3.716 (25)             | 0.92                        |
| 2,3,4,5,6-Pentachlorotoluene                              | 4.8 (20)                          |                             |
| Pentadecane                                               |                                   | 0                           |
| <i>cis</i> -1,3-Pentadiene                                | 2.32 (25)                         | 0.50 (25, B)                |
| 1,4-Pentadiene                                            | 2.054 (24)                        |                             |
| Pentanal                                                  | 10.1 (17), 10.00 (20)             | 2.59 (20, B)                |
| Pentane                                                   | 2.011 (–90), 1.837 (20)           | 0                           |
| 1,2-Pentanediol                                           | 17.31 (24)                        |                             |
| 1,4-Pentanediol                                           | 26.74 (23)                        |                             |
| 1,5-Pentanediol                                           | 26.2 (20)                         | 2.45 (20, D)                |
| 2,3-Pentanediol                                           | 17.37 (24)                        |                             |
| 2,4-Pentanediol                                           | 24.69 (21)                        |                             |
| 2,4-Pentanedione                                          | 26.52 (30)                        | 3.03                        |
| Pentanenitrile                                            | 20.04 (20)                        | 4.12, 3.57 (25, B)          |
| 1-Pentanethiol                                            | 4.85 (20), 4.55 (25), 4.23 (50)   | 1.54 (25, lq)               |
| Pentanoic acid                                            | 2.66 (21)                         | 1.61 (20, D)                |
| 1-Pentanol                                                | 16.9 (20), 15.13 (25)             | 1.71 (20, B)                |
| 2-Pentanol                                                | 13.71 (25)                        | 1.66 (22, B)                |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                    | Dielectric constant, $\epsilon$  | Dipole moment, D |
|------------------------------|----------------------------------|------------------|
| 3-Pentanol                   | 13.35 (25)                       | 1.64 (22, B)     |
| 2-Pentanone                  | 15.45 (20), 11.73 (80)           | 2.72 (22, B)     |
| 3-Pentanone                  | 19.4 (– 20), 17.00 (20)          | 2.72 (20, B)     |
| 2-Pentanone oxime            | 3.3 (25)                         |                  |
| 1-Pentene                    | 2.011 (20)                       | 0.5              |
| <i>cis</i> -2-Pentene        |                                  | 0                |
| <i>trans</i> -2-Pentene      |                                  | 0                |
| Pentyl acetate               | 4.79 (20)                        | 1.75             |
| Pentylamine                  | 4.27 (20)                        | 1.55 (30, B)     |
| Pentyl formate               | 5.7 (19)                         | 1.90             |
| Pentyl nitrate               | 9.0 (18)                         |                  |
| Pentyl nitrite               | 7.21 (25)                        |                  |
| <i>tert</i> -Pentyl nitrite  | 10.88 (25)                       |                  |
| Phenanthrene                 | 2.8 (20)                         | 0                |
| Phenol                       | 12.40 (30), 9.78 (60)            | 1.224            |
| Phenoxyacetylene             | 4.76 (25)                        | 1.42 (25, lq)    |
| Phenyl acetate               | 5.40 (25)                        | 1.54 (22, B)     |
| Phenylacetic acid            | 3.47 (80)                        |                  |
| Phenylacetonitrile           | 17.87 (26), 8.5 (234)            | 3.47 (27, B)     |
| Phenylacetylene              | 2.98 (20)                        | 0.72 (20, B)     |
| 1-Phenylethanol              | 8.77 (20), 7.6 (90)              | 1.51 (20, B)     |
| 2-Phenylethanol              | 12.31 (20)                       |                  |
| Phenylhydrazine              | 7.15 (20)                        | 1.67 (25, B)     |
| Phenyl isocyanate            | 8.94 (20)                        |                  |
| Phenyl isothiocyanate        | 10 (20)                          |                  |
| 1-Phenylpropene              | 2.7 (20)                         |                  |
| 2-Phenylpropene              | 2.3 (20)                         |                  |
| 3-Phenylpropene              | 2.6 (20)                         |                  |
| Phenyl salicylate            | 6.3 (50)                         |                  |
| Phosgene                     | 4.7 (0), 4.3 (22)                |                  |
| Phthalide                    | 36 (75)                          |                  |
| ( $\pm$ )- $\alpha$ -Pinene  | 2.64 (25), 2.26 (30)             | 0.60 (25, B)     |
| L- $\beta$ -Pinene           | 2.76 (20)                        |                  |
| Piperidine                   | 4.33 (20)                        | 1.19 (25, B)     |
| Propanal                     | 18.5 (17)                        | 2.52             |
| Propane                      | 1.668 (20)                       | 0.084            |
| 1,2-Propanediamine           | 10.2                             |                  |
| 1,3-Propanediamine           | 9.55                             | 1.96 (25, B)     |
| 1,2-Propanediol              | 32.0 (20), 27.5 (30)             | 2.27 (25, D)     |
| 1,3-Propanediol              | 35.1 (20)                        | 2.52 (25, D)     |
| 1,2-Propanediol dinitrate    | 26.80 (20)                       |                  |
| 1,3-Propanediol dinitrate    | 18.97 (20)                       |                  |
| 1,2-Propanedithiol           | 7.24 (20)                        |                  |
| 1,3-Propanedithiol           | 8.11 (30)                        |                  |
| Propanenitrile               | 29.7 (20)                        | 4.05             |
| 1-Propanethiol               | 5.94 (15), 1.55 (25)             | 1.68             |
| 2-Propanethiol               | 5.95 (25)                        | 1.61             |
| 1,2,3-Propanetriol 1-acetate | 38.57 (– 31), 7.11 (20)          |                  |
| Propanoic acid               | 3.30 (10), 3.44 (25)             | 1.76             |
| Propanoic anhydride          | 18.30 (20)                       |                  |
| 1-Propanol                   | 20.8 (20), 20.33 (25)            | 1.55             |
| 2-Propanol                   | 20.18 (20), 18.3 (25), 16.2 (40) | 1.58             |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                            | Dielectric constant, $\epsilon$    | Dipole moment, D                           |
|--------------------------------------|------------------------------------|--------------------------------------------|
| 2-Propenal                           |                                    | 3.12                                       |
| Propene                              | 2.137 (– 53), 1.88 (20), 1.44 (90) | 0.366                                      |
| Propenenitrile                       | 33.0 (20)                          | 3.87                                       |
| 2-Propen-1-ol                        | 21.6 (15), 19.7 (20)               | 1.60                                       |
| Propionaldehyde (propanal)           | 18.5 (17)                          | 2.75                                       |
| Propionamide                         |                                    | 3.4 (30, B)                                |
| Propyl acetate                       | 5.62 (20)                          | 1.86 (25, B)                               |
| <i>N</i> -Propylacetamide            | 117.8 (25)                         |                                            |
| Propylamine                          | 5.31 (20), 5.08 (26)               | 1.17                                       |
| Propylbenzene                        | 2.37 (20), 2.351 (30)              | 0                                          |
| Propyl benzoate                      | 5.78 (30)                          |                                            |
| Propyl butanoate                     | 4.3 (20)                           |                                            |
| Propyl carbamate                     | 12.06 (65)                         |                                            |
| Propylene carbonate                  | 66.14 (20)                         | 4.9                                        |
| Propyleneimine                       |                                    | 1.77 ( <i>cis</i> ), 1.60 ( <i>trans</i> ) |
| 1,2-Propylene oxide                  |                                    | 2.00                                       |
| Propyl formate                       | 7.72 (19), 6.92 (30)               | 1.91 (22, B)                               |
| Propyl nitrate                       | 14 (18)                            | 3.01 (20, B)                               |
| Propyl nitrite                       | 12.35 (– 23)                       |                                            |
| Propyl pentanoate                    | 4 (19)                             |                                            |
| <i>N</i> -Propylpropanamide          | 118.1 (25)                         |                                            |
| Propyl propanoate                    | 5.25 (20)                          | 1.79 (22, B)                               |
| Propyl trichloroacetate              | 8.32 (25)                          |                                            |
| Propyne                              | 3.218 (– 27)                       | 0.784                                      |
| 2-Propyn-1-ol                        | 20.8 (20)                          | 1.13                                       |
| Pulegone                             | 9.5 (20)                           | 2.00 (25, B)                               |
| Pyridazine                           |                                    | 4.22                                       |
| Pyrazine                             | 2.80 (50)                          | 0                                          |
| Pyridine                             | 13.26 (20), 12.3 (25), 9.4 (116)   | 2.215                                      |
| Pyridine-1-oxide                     | 35.94 (70)                         |                                            |
| Pyrimidine                           |                                    | 2.33                                       |
| 1 <i>H</i> -Pyrrole                  | 8.00 (20), 8.13 (25)               | 1.74                                       |
| Pyrrolidine                          | 8.30 (20)                          | 1.58 (20, B)                               |
| 2-Pyrrolidone                        |                                    | 3.55 (25, B)                               |
| Quinoline                            | 9.16 (20), 9.00 (25)               | 2.29                                       |
| Safrole                              | 3.1 (21)                           |                                            |
| Salicylaldehyde                      | 18.35 (20)                         | 2.86 (20, B)                               |
| <b>D</b> -Sorbitol                   | 35.5 (80)                          |                                            |
| Squalane                             | 1.911 (100)                        | 0                                          |
| Squalene                             |                                    | 0.68 (25, B)                               |
| Stearic acid                         | 2.29 (70), 2.26 (100)              | 1.76 (25, D)                               |
| Styrene                              | 2.47 (20), 2.43 (25), 2.32 (75)    | 0.13 (25, lq)                              |
| Succinonitrile                       | 62.6 (25), 56.5 (57), 54 (68)      | 3.68 (30, toluene)                         |
| $\alpha$ -Terpinene                  | 2.45 (25)                          |                                            |
| Terpinolene                          | 2.29 (25)                          |                                            |
| 1,1,2,2-Tetrabromoethane             | 8.6 (3), 7.0 (22), 6.72 (30)       | 1.41                                       |
| 1,1,2,2-Tetrachlorodifluoroethane    | 2.52 (35)                          |                                            |
| 1,1,1,2-Tetrachloroethane            | 9.22 (– 66)                        |                                            |
| 1,1,2,2-Tetrachloroethane            | 8.50 (20)                          | 1.32                                       |
| Tetrachloroethylene                  | 2.30 (25), 2.268 (30)              | 0                                          |
| 1,1,3,4-Tetrachlorohexafluoro-butane | 2.86 (20)                          |                                            |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                      | Dielectric constant, $\epsilon$ | Dipole moment, D |
|------------------------------------------------|---------------------------------|------------------|
| Tetradecafluorohexane                          | 1.76 (25)                       |                  |
| Tetradecamethylhexasiloxane                    | 2.5 (20)                        | 1.58 (20, lq)    |
| Tetradecane                                    |                                 | 0                |
| Tetradecanoic acid                             |                                 | 0.76 (25, B)     |
| 1-Tetradecanol                                 | 4.72 (38), 4.40 (48)            | 1.69 (25, C)     |
| Tetraethylene glycol                           | 20.44 (20)                      | 5.84 (20, lq)    |
| Tetraethyl lead                                |                                 | 0.3 (20, B)      |
| Tetraethylsilane                               | 2.09 (20)                       | 0                |
| Tetraethyl silicate                            | 4.1 (20)                        | 1.72 (32, B)     |
| Tetrafluoromethane                             | 1.685 (– 147)                   |                  |
| 2,2,3,3-Tetrafluoro-1-propanol                 | 21.03 (25)                      |                  |
| Tetrahydrofuran                                | 11.6 (– 70), 7.52 (22)          | 1.75 (25, B)     |
| Tetrahydro-2-furanmethanol                     | 13.61 (23), 13.48 (30)          | 2.12 (35, lq)    |
| 2-Tetrahydrofurfuryl acetate                   | 9.65 (20)                       |                  |
| 1,2,3,4-Tetrahydronaphthalene                  | 2.77 (25)                       | 0                |
| 1,2,3,4-Tetrahydro-2-naphthol                  | 11.7 (20), 6.7 (90)             |                  |
| Tetrahydropyran                                | 5.66 (20), 5.61 (25)            | 1.74             |
| Tetrahydrothiophene                            |                                 | 1.9              |
| Tetrahydrothiophene-1,1-dioxide<br>(sulfolane) | 43.26 (30)                      | 4.81 (25, B)     |
| Tetrahydrothiophene-S-oxide                    | 42.96 (25), 42.5 (30)           |                  |
| Tetrakis(methylthio)methane                    | 2.818 (70)                      |                  |
| Tetramethoxymethane                            | 2.40 (20)                       |                  |
| Tetramethyl germanium                          | 1.817 (24)                      |                  |
| 1,1,3,3-Tetramethylguanidine                   | 11.5 (25)                       |                  |
| Tetramethylsilane                              | 1.921 (20)                      | 0                |
| Tetramethyl silicate                           | 6.0 (20)                        |                  |
| 1,1,2,2-Tetramethylurea                        | 23.10 (20)                      | 3.47 (25, B)     |
| Tetranitromethane                              | 2.317 (25)                      | 0                |
| Tetrathiomethylmethane                         | 2.82 (70)                       |                  |
| Thiacyclopentane                               |                                 | 1.90 (25, B)     |
| Thioacetic acid                                | 14.30 (25)                      |                  |
| Thiophene                                      | 2.74 (20), 2.57 (25)            | 0.55             |
| Thymol                                         |                                 | 1.55 (25, B)     |
| Toluene                                        | 2.385 (20), 2.364 (30)          | 0.375            |
| <i>o</i> -Toluidine                            | 6.34 (18), 6.14 (25), 5.71 (58) | 1.60 (25, B)     |
| <i>m</i> -Toluidine                            | 5.95 (18), 5.82 (25), 5.45 (58) | 1.45 (25, B)     |
| <i>p</i> -Toluidine                            | 5.06 (60)                       | 1.52 (25, B)     |
| <i>m</i> -Tolunitrile                          |                                 | 4.21 (22, B)     |
| <i>p</i> -Tolunitrile                          |                                 | 4.47 (20, B)     |
| Tribenzylamine                                 |                                 | 0.65 (20, B)     |
| 2,2,2-Tribromoacetaldehyde                     | 7.6 (20)                        | 1.70 (20, C)     |
| Tribromochloromethane                          | 2.60 (60)                       |                  |
| Tribromofluoromethane                          | 3.00 (20)                       |                  |
| Tribromomethane                                | 4.404 (10), 4.39 (20)           | 0.99             |
| Tribromonitromethane                           | 9.03 (25)                       |                  |
| 1,2,3-Tribromopropane                          | 6.45 (20), 6.00 (30)            | 1.59 (25, B)     |
| Tributylamine                                  | 2.34 (20)                       | 0.78 (25, B)     |
| Tributyl borate                                | 2.23 (20)                       | 0.78 (25, C)     |
| Tributyl phosphate                             | 8.34 (20), 7.96 (30)            | 3.07 (25, B)     |
| Tributyl phosphite                             |                                 | 1.92 (20, C)     |
| Trichloroacetaldehyde                          | 7.6 (– 40), 6.9 (20), 6.8 (25)  | 1.96 (25, B)     |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                                | Dielectric constant, $\epsilon$    | Dipole moment, D            |
|------------------------------------------|------------------------------------|-----------------------------|
| Trichloroacetic acid                     | 4.34 (60)                          | 1.1 (25, B, dimer)          |
| Trichloroacetic anhydride                | 5.0 (25)                           |                             |
| Trichloroacetoneitrile                   | 7.85 (19)                          | 1.93 (19, lq)               |
| 4,4,4-Trichlorobutanal                   | 10.0 (18)                          |                             |
| 1,2,2-Trichloro-1,1-difluoroethane       | 4.01 (30)                          |                             |
| 1,1,1-Trichloroethane                    | 7.1 (7), 7.24 (20)                 | 1.755                       |
| 1,1,2-Trichloroethane                    | 7.19 (25)                          | 1.45                        |
| Trichloroethylene                        | 3.42 (16), 3.39 (28)               | 0.77 (30, lq), 0.95 (30, B) |
| Trichloroethylsilane                     |                                    | 2.0                         |
| Trichlorofluoromethane                   | 3.00 (25), 2.28 (29)               | 0.45                        |
| (Trichloromethyl)benzene                 | 6.9 (21)                           | 2.0                         |
| Trichloromethylsilane                    |                                    | 1.87 (25, B)                |
| Trichloronitromethane                    | 7.32 (25)                          |                             |
| 2,4,6-Trichlorophenol                    |                                    | 1.88 (25, D)                |
| 1,2,3-Trichloropropane                   | 7.5 (20)                           | 1.61                        |
| Trichlorosilane                          |                                    | 0.86                        |
| $\alpha,\alpha,\alpha$ -Trichlorotoluene | 6.9 (21)                           | 2.17 (20, B)                |
| 1,1,2-Trichloro-1,2,2-trifluoroethane    | 2.41 (25)                          |                             |
| Tridecane                                | 2.02 (20)                          | 0                           |
| 1-Tridecene                              | 2.14 (20)                          | 0                           |
| Triethanolamine                          | 29.36 (25)                         | 3.57 (25, B)                |
| Triethoxymethane                         | 4.779 (20)                         |                             |
| Triethylaluminum                         | 2.9 (20)                           |                             |
| Triethylamine                            | 2.418 (20)                         | 0.66                        |
| Triethylborane                           | 1.874 (20)                         |                             |
| Triethylene glycol                       | 23.69 (20)                         | 5.58 (20, lq)               |
| Triethylenetetramine                     | 10.76 (20)                         |                             |
| Triethyl orthovanadate                   | 3.333 (25)                         |                             |
| Triethyl phosphate                       | 13.43 (15), 13.20 (25), 10.93 (65) | 3.08 (25, B)                |
| Triethylphosphine oxide                  | 35.5 (50)                          |                             |
| Triethylphosphine sulfide                | 39.0 (98)                          |                             |
| Triethyl phosphite                       | 5.0                                | 1.82 (25, D)                |
| Trifluoroacetic acid                     | 8.42 (20), 5.76 (50)               | 2.28                        |
| Trifluoroacetic anhydride                | 2.7 (25)                           |                             |
| 1,1,1-Trifluoroethane                    |                                    | 2.347                       |
| 2,2,2-Trifluoroethanol                   | 27.68 (20)                         | 2.03 (25, cHex)             |
| Trifluoromethane                         | 5.2 (26)                           | 1.651                       |
| (Trifluoromethyl)benzene                 | 9.22 (25)                          | 2.86                        |
| 1-Trifluoromethyl-3-nitrobenzene         | 17.0 (30)                          |                             |
| $\alpha,\alpha,\alpha$ -Trifluorotoluene | 9.2 (30), 8.1 (60)                 |                             |
| Trimethoxymethylsilane                   | 4.9 (25)                           |                             |
| Trimethylamine                           | 2.44 (25)                          | 0.612                       |
| 1,2,3-Trimethylbenzene                   | 2.66 (20), 2.609 (30)              | 0                           |
| 1,2,4-Trimethylbenzene                   | 2.38 (20), 2.36 (30)               | 0                           |
| 1,3,5-Trimethylbenzene                   | 2.28 (20)                          | 0                           |
| Trimethyl borate                         | 2.276 (20)                         | 0.82 (25, C)                |
| 2,2,3-Trimethylbutane                    | 1.930 (20)                         | 0                           |
| Trimethylchlorosilane                    | 10.21 (0)                          |                             |
| Trimethylene sulfide                     |                                    | 1.85                        |
| 2,2,5-Trimethylhexane                    |                                    | 0                           |
| 2,3,5-Trimethylhexane                    |                                    | 0                           |
| 2,2,3-Trimethylpentane                   | 1.962 (20)                         | 0                           |

**TABLE 5.17** Dielectric Constant (Permittivity) and Dipole Moment of Various Organic Substances (*Continued*)

| Substance                        | Dielectric constant, $\epsilon$ | Dipole moment, D            |
|----------------------------------|---------------------------------|-----------------------------|
| 2,2,4-Trimethylpentane           | 1.940 (20)                      | 0                           |
| 2,3,3-Trimethylpentane           | 1.98 (20)                       | 0                           |
| 2,3,4-Trimethylpentane           | 1.97 (20)                       | 0                           |
| Trimethyl phosphate              | 20.6 (20)                       | 3.2                         |
| Trimethylphosphine sulfide       |                                 | 71.6 (20)                   |
| Trimethyl phosphite              |                                 | 1.83 (20, C)                |
| 2,4,6-Trimethylpyridine          | 7.807 (25)                      | 1.95 (25, B)                |
| 2,4,6-Trinitrophenol             | 4.0 (21)                        |                             |
| 1,3,5-Trioxane                   | 15.55 (65)                      | 2.08                        |
| Triphenyl phosphite              | 3.67 (45), 3.57 (65)            | 2.04 (25, B)                |
| Tris(4-ethylphenyl) phosphite    | 3.74 (15), 3.61 (45)            | 2.08 (25, B)                |
| Tris(2-methylphenyl) phosphate   | 6.7 (25)                        | 2.9                         |
| Tris(3-methylphenyl) phosphate   |                                 | 3.0                         |
| Tris(4-methylphenyl) phosphate   |                                 | 3.2                         |
| Tris( <i>m</i> -tolyl) phosphite | 3.67 (15), 3.53 (45)            | 1.62 (25, B)                |
| Tris( <i>p</i> -tolyl) phosphite | 3.88 (15), 3.74 (45)            | 1.77 (25, B)                |
| Tri- <i>o</i> -tolyl phosphate   | 6.92 (40)                       | 2.84 (40, C)                |
| Undecane                         | 2.00 (20), 1.84 (150)           | 0                           |
| 2-Undecanone                     |                                 | 2.71 (15, B)                |
| 1-Undecene                       | 2.14 (20)                       | 0                           |
| Urea                             |                                 | 4.59 (25, D)                |
| Vinyl acetate                    |                                 | 1.79 (25, B)                |
| Vinyl chloride                   | 6.26 (17)                       | 1.45                        |
| Vinyl isocyanate                 | 10.62 (25)                      |                             |
| 2-Vinylpyridine                  | 9.126 (20)                      |                             |
| 4-Vinylpyridine                  | 10.50 (20)                      |                             |
| <i>o</i> -Xylene                 | 2.562 (20), 2.54 (30)           | 0.62                        |
| <i>m</i> -Xylene                 | 2.359 (20), 2.35 (30)           | 0.33 (20, lq), 0.37 (20, B) |
| <i>p</i> -Xylene                 | 2.273 (20), 2.22 (50)           | 0                           |
| Xylitol                          | 40.0 (20)                       |                             |

**TABLE 5.18** Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances

For the majority of compounds the dependence of the surface tension  $\gamma$  on the temperature can be given as:

$$\gamma = a - bt$$

where  $a$  and  $b$  are constants and  $t$  is the temperature in degrees Celsius.  
The values of the dipole moment are for the gas phase.

| Substance                                    | Viscosity,<br>$\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$     | Dielectric<br>constant, $\epsilon$                   | Dipole<br>moment, D | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |                    |
|----------------------------------------------|------------------------------------------------------------------|------------------------------------------------------|---------------------|-----------------------------------------------------|--------------------|
|                                              |                                                                  |                                                      |                     | $a$                                                 | $b$                |
| Air                                          | 0.0182 <sup>20</sup> ,<br>0.0231 <sup>127</sup>                  | 1.000 536 4                                          |                     |                                                     |                    |
| AlBr <sub>3</sub>                            |                                                                  | 3.38 <sup>100</sup>                                  | 5.2                 |                                                     |                    |
| Ar                                           |                                                                  |                                                      |                     |                                                     |                    |
| (g)                                          | 0.0233 <sup>20</sup> ,<br>0.0288 <sup>127</sup>                  | 1.000 517 2                                          |                     |                                                     |                    |
| (lq)                                         |                                                                  | 1.538 <sup>-191</sup> ,<br>1.325 <sup>-132</sup>     | 0                   | 34.28                                               | 0.2493             |
| AsBr <sub>3</sub>                            |                                                                  | 8.83 <sup>35</sup>                                   | 1.61                | 54.41                                               | 0.1043             |
| AsCl <sub>3</sub>                            |                                                                  | 12.6 <sup>20</sup>                                   | 1.59                | 41.67                                               | 0.097 81           |
| AsH <sub>3</sub> (arsine)                    |                                                                  | 2.40 <sup>-72</sup> , 2.05 <sup>20</sup>             | 0.20                |                                                     |                    |
| BBr <sub>3</sub>                             |                                                                  | 2.58 <sup>0</sup>                                    | 0                   | 31.90                                               | 0.1280             |
| BCl <sub>3</sub>                             |                                                                  |                                                      | 0                   |                                                     |                    |
| BF <sub>3</sub>                              | 0.0171 <sup>27</sup> ,<br>0.0217 <sup>127</sup>                  |                                                      | 0                   | - 2.92                                              | 0.2030             |
| B <sub>2</sub> H <sub>6</sub> (diborane)     |                                                                  | 1.872 <sup>-92.5</sup>                               | 0                   | - 3.13                                              | 0.1783             |
| B <sub>4</sub> H <sub>10</sub>               |                                                                  |                                                      | 0.486               |                                                     |                    |
| B <sub>5</sub> H <sub>9</sub>                |                                                                  | 21.1 <sup>25</sup>                                   | 2.13                |                                                     |                    |
| B <sub>6</sub> H <sub>10</sub>               |                                                                  |                                                      | 2.50                |                                                     |                    |
| B <sub>3</sub> H <sub>6</sub> N <sub>3</sub> |                                                                  |                                                      | 0                   |                                                     |                    |
| Br <sub>2</sub> (g)                          |                                                                  | 1.0128 <sup>20</sup>                                 |                     |                                                     |                    |
| (lq)                                         | 1.252 <sup>0</sup> , 1.03 <sup>16</sup> ,<br>0.744 <sup>25</sup> | 3.1484 <sup>25</sup>                                 | 0                   | 45.5                                                | 0.1820             |
| BrF <sub>3</sub>                             | 2.22 <sup>20</sup>                                               | 106.8 <sup>25</sup>                                  | 1.1                 | 38.30                                               | 0.0999             |
| BrF <sub>5</sub>                             | 0.62 <sup>24</sup>                                               | 7.91 <sup>24.5</sup>                                 | 1.51                | 25.24                                               | 0.1098             |
| Cl <sub>2</sub> (g)                          | 0.0132 <sup>20</sup>                                             |                                                      | 0                   |                                                     |                    |
| (lq)                                         |                                                                  | 2.147 <sup>-65</sup> ,<br>1.91 <sup>14</sup>         |                     | 19.87                                               | 0.1897             |
| ClF <sub>3</sub>                             | 0.48 <sup>12</sup>                                               | 4.394 <sup>20</sup> , 4.29 <sup>25</sup>             | 0.554               | 26.9                                                | 0.1660             |
| ClF <sub>5</sub>                             |                                                                  | 4.28 <sup>-80</sup>                                  |                     |                                                     |                    |
| ClO <sub>3</sub> F                           |                                                                  | 2.194 <sup>-123</sup>                                | 0.023               | 12.24                                               | 0.1576             |
| CO (g)                                       | 0.0175 <sup>20</sup> ,<br>0.0221 <sup>127</sup>                  | 1.000 70 <sup>0</sup>                                | 0.112               |                                                     |                    |
| (lq)                                         |                                                                  |                                                      |                     | - 30.20                                             | 0.2073             |
| CO <sub>2</sub> (g)                          | 0.0147 <sup>20</sup> ,<br>0.0197 <sup>127</sup>                  | 1.000 922                                            | 0                   |                                                     |                    |
| (lq)                                         | 0.071 <sup>20</sup>                                              | 1.60 <sup>0°C, 50 atm</sup> ,<br>1.449 <sup>23</sup> |                     | 6.14 <sup>-10</sup>                                 | 2.67 <sup>10</sup> |
| COCl <sub>2</sub>                            |                                                                  | 4.34 <sup>22</sup>                                   | 1.17                | 22.59                                               | 0.1456             |
| COF <sub>2</sub>                             |                                                                  |                                                      | 0.95                |                                                     |                    |
| COS                                          |                                                                  | 4.47 <sup>-88</sup>                                  | 0.712               | 12.12                                               | 0.1779             |
| COSe                                         |                                                                  | 3.47 <sup>10</sup>                                   | 0.73                |                                                     |                    |
| CS                                           |                                                                  |                                                      | 1.98                |                                                     |                    |

**TABLE 5.18** Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*Continued*)

| Substance                                                                                              | Viscosity,<br>mN · s · m <sup>-2</sup>                                 | Dielectric<br>constant, $\epsilon$                                                  | Dipole<br>moment, D           | Surface tension,<br>mN · m <sup>-1</sup>                                      |                                                                               |
|--------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
|                                                                                                        |                                                                        |                                                                                     |                               | <i>a</i>                                                                      | <i>b</i>                                                                      |
| CS <sub>2</sub> (g)<br>(lq)                                                                            | 0.429 <sup>0</sup> , 0.375 <sup>20</sup> ,<br>0.352 <sup>25</sup>      | 1.0029 <sup>0</sup><br>2.632 <sup>20</sup>                                          | 0                             | 35.29                                                                         | 0.1484                                                                        |
| CrO <sub>2</sub> Cl <sub>2</sub><br>D <sub>2</sub> (deuterium)                                         | 0.0126 <sup>27</sup> ,<br>0.0154 <sup>127</sup>                        | 2.6 <sup>20</sup><br>1.290 <sup>-255</sup> ,<br>1.277 <sup>-253</sup>               | 0.47                          |                                                                               |                                                                               |
| DH<br>D <sub>2</sub> O                                                                                 | 0.0111 <sup>25</sup> (g),<br>1.098 <sup>25</sup> (lq)                  | 1.269 <sup>16.78 K</sup><br>79.75 <sup>20</sup> ,<br>78.25 <sup>25</sup>            | 1.87                          | 6.537<br>71.72 <sup>20</sup>                                                  | 0.1883<br>68.38 <sup>40</sup>                                                 |
| F <sub>2</sub>                                                                                         |                                                                        | 1.491 <sup>-220</sup> ,<br>1.54 <sup>-202</sup>                                     |                               | - 16.10                                                                       | 0.1646                                                                        |
| GaCl <sub>3</sub><br>GeBr <sub>4</sub><br>GeBr <sub>4</sub><br>GeCl <sub>4</sub><br>GeClH <sub>3</sub> |                                                                        |                                                                                     | 0.85                          | 35.0<br>35.51 <sup>30</sup><br>35.51 <sup>30</sup><br>22.44 <sup>30</sup>     | 0.1000<br>33.70 <sup>50</sup><br>33.70 <sup>50</sup>                          |
| H <sub>2</sub> (g)<br>t                                                                                | 0.0088 <sup>20</sup> ,<br>0.109 <sup>127</sup>                         | 2.463 <sup>0</sup> , 2.430 <sup>25</sup>                                            | 0                             |                                                                               |                                                                               |
| (lq)                                                                                                   |                                                                        | 1.000 253 8                                                                         | 2.13<br>0                     |                                                                               |                                                                               |
| HBr (g)<br>(lq)                                                                                        |                                                                        | 1.279 <sup>13.5 K</sup> ,<br>1.228 <sup>20.4 K</sup>                                | 0.827                         | 2.80 <sup>-258</sup>                                                          | 2.12 <sup>-254</sup>                                                          |
| He (g)                                                                                                 | 0.83 <sup>-67</sup><br>0.0196 <sup>27</sup> ,<br>0.0244 <sup>27</sup>  | 1.003 13 <sup>0</sup><br>8.23 <sup>-86</sup> , 3.82 <sup>25</sup><br>1.000 065 0    | 0                             | 13.10                                                                         | 0.2079                                                                        |
| (lq) (II)<br>(III)<br>(IV)                                                                             |                                                                        | 1.0555 <sup>2.055 K</sup>                                                           |                               | 0.351 <sup>0.50 K</sup><br>0.151 <sup>3.61 K</sup><br>0.372 <sup>0.50 K</sup> | 0.317 <sup>2.00 K</sup><br>0.131 <sup>1.13 K</sup><br>0.354 <sup>1.40 K</sup> |
| HCl (g)<br>(lq)                                                                                        | 0.0146 <sup>27</sup> ,<br>0.0197 <sup>127</sup><br>0.51 <sup>-95</sup> | 1.0046 <sup>0</sup><br>14.3 <sup>-114</sup> ,<br>4.60 <sup>28</sup>                 | 1.109                         |                                                                               |                                                                               |
| HClO<br>HCN                                                                                            |                                                                        |                                                                                     | 1.3<br>2.98                   | 19.45 <sup>10</sup>                                                           | 18.33 <sup>20</sup>                                                           |
| HCNO (iso-<br>cyanate)                                                                                 |                                                                        |                                                                                     | 1.6                           |                                                                               |                                                                               |
| HCNS<br>HF<br>HFO<br>HI (g)<br>(lq)<br>HN <sub>3</sub> (azide)<br>H <sub>2</sub> O (see Table<br>5.19) | 0.256 <sup>0</sup>                                                     | 83.6 <sup>0</sup>                                                                   | 1.7<br>1.826<br>2.23<br>0.448 | 10.41                                                                         | 0.078 67                                                                      |
| H <sub>2</sub> O <sub>2</sub><br>HNO <sub>3</sub><br>H <sub>2</sub> S (g)<br>(lq)<br>H <sub>2</sub> Se | 1.25 <sup>20</sup><br>0.412 <sup>0</sup>                               | 84.2 <sup>0</sup> , 74.6 <sup>17</sup><br>1.0040 <sup>0</sup><br>5.93 <sup>10</sup> | 1.573<br>2.17<br>0.97<br>0.24 | 78.97<br>48.95<br>22.32                                                       | 0.1549<br>0.1758<br>0.1482                                                    |



**TABLE 5.18** Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*Continued*)

| Substance                                      | Viscosity,<br>mN · s · m <sup>-2</sup>                             | Dielectric<br>constant, $\epsilon$                 | Dipole<br>moment, D | Surface tension,<br>mN · m <sup>-1</sup> |                      |
|------------------------------------------------|--------------------------------------------------------------------|----------------------------------------------------|---------------------|------------------------------------------|----------------------|
|                                                |                                                                    |                                                    |                     | <i>a</i>                                 | <i>b</i>             |
| HSO <sub>3</sub> Cl                            | 2.43 <sup>20</sup>                                                 | 60 <sup>60</sup>                                   |                     |                                          |                      |
| HSO <sub>3</sub> F                             | 1.56 <sup>25</sup>                                                 | ca. 120 <sup>25</sup>                              |                     |                                          |                      |
| H <sub>2</sub> SO <sub>4</sub>                 | 24.54 <sup>25</sup>                                                | 100 <sup>25</sup>                                  |                     |                                          |                      |
| H <sub>2</sub> Te                              |                                                                    |                                                    | <0.2                | 29.03                                    | 0.2619               |
| Hg                                             | 1.552 <sup>20</sup> , 1.526 <sup>25</sup> ,<br>1.402 <sup>50</sup> |                                                    | 0                   | 490.6                                    | 0.2049               |
| I <sub>2</sub>                                 | 1.98 <sup>116</sup>                                                | 11.1 <sup>118</sup>                                | 0                   |                                          |                      |
| IBr                                            |                                                                    |                                                    | 0.726               |                                          |                      |
| IF                                             |                                                                    |                                                    | 1.95                |                                          |                      |
| IF <sub>5</sub>                                |                                                                    | 37.13 <sup>20</sup>                                | 2.18                | 33.16                                    | 0.1318               |
| IF <sub>7</sub>                                |                                                                    | 1.97 <sup>23</sup>                                 |                     |                                          |                      |
| IOF <sub>5</sub>                               |                                                                    | 1.75 <sup>25</sup>                                 |                     |                                          |                      |
| Kr (g)                                         | 0.0250 <sup>20</sup> ,<br>0.0331 <sup>127</sup>                    |                                                    | <0.05               |                                          |                      |
| (lq)                                           |                                                                    | 1.644 <sup>-153.4</sup>                            |                     | 40.576 (in K)                            | 0.2890 (in K)        |
| Mn <sub>2</sub> O <sub>7</sub>                 |                                                                    | 3.28 <sup>20</sup>                                 |                     |                                          |                      |
| Ne (g)                                         | 0.0303 <sup>20</sup> ,<br>0.0389 <sup>127</sup>                    | 1.000 063 9 <sup>20</sup>                          | 0                   |                                          |                      |
| (lq)                                           |                                                                    | 1.1907 <sup>-247.1</sup>                           |                     |                                          |                      |
| N <sub>2</sub> (g)                             | 0.0176 <sup>20</sup> ,<br>0.0222 <sup>127</sup>                    | 1.000 548 0 <sup>20</sup>                          | 0                   |                                          |                      |
| (lq)                                           |                                                                    | 1.468 <sup>-210</sup> ,<br>1.454 <sup>-203</sup>   |                     | 26.42 (in K)                             | 0.2265 (in K)        |
| NH <sub>3</sub> (g)                            |                                                                    | 1.007 <sup>20</sup>                                | 1.471               |                                          |                      |
| (lq)                                           | 0.254 <sup>-33.5</sup>                                             | 22.4 <sup>-33.5</sup> ,<br>16.61 <sup>20</sup>     |                     | 37.91 <sup>-50</sup>                     | 35.38 <sup>-40</sup> |
| N <sub>2</sub> H <sub>4</sub> (hydra-<br>zine) | 0.97 <sup>20</sup> , 0.876 <sup>25</sup> ,<br>0.628 <sup>50</sup>  | 52.9 <sup>20</sup> , 51.7 <sup>25</sup>            | 1.75                | 72.41                                    | 0.2407               |
| Ni(CO) <sub>4</sub>                            |                                                                    |                                                    |                     | 18.11                                    | 0.1117               |
| NO                                             | 0.0192 <sup>27</sup> ,<br>0.0238 <sup>127</sup>                    |                                                    | 0.159               | -67.48                                   | 0.5853               |
| N <sub>2</sub> O (g)                           | 0.0146 <sup>20</sup> ,<br>0.0194 <sup>127</sup>                    | 1.001 13 <sup>0</sup>                              | 0.161               |                                          |                      |
| (lq)                                           |                                                                    | 1.52 <sup>15</sup>                                 |                     | 5.09                                     | 0.2032               |
| NO <sub>2</sub>                                | 0.532 <sup>0</sup> , 0.402 <sup>25</sup>                           |                                                    | 0.316               |                                          |                      |
| N <sub>2</sub> O <sub>4</sub>                  |                                                                    | 2.56 <sup>25</sup> , 2.44 <sup>20</sup>            | 0.5                 |                                          |                      |
| N <sub>2</sub> O <sub>3</sub>                  |                                                                    |                                                    | 2.122               |                                          |                      |
| NOBr                                           |                                                                    | 13.4 <sup>15</sup>                                 | 1.8                 |                                          |                      |
| NOCl                                           |                                                                    | 18.2 <sup>12</sup>                                 | 1.9                 | 29.49                                    | 0.1493               |
| NO <sub>2</sub> Cl                             |                                                                    |                                                    | 0.53                |                                          |                      |
| NOF                                            |                                                                    |                                                    | 1.73                | 14.00                                    | 0.1165               |
| NO <sub>2</sub> F                              |                                                                    |                                                    | 0.47                | 8.26                                     | 0.1854               |
| NO <sub>3</sub>                                |                                                                    | 31.13 <sup>-70</sup>                               |                     |                                          |                      |
| O <sub>2</sub> (g)                             | 0.0204 <sup>20</sup> ,<br>0.0261 <sup>127</sup>                    | 1.000 494 7 <sup>20</sup>                          | 0                   |                                          |                      |
| (lq)                                           |                                                                    | 1.568 <sup>-218.7</sup> ,<br>1.507 <sup>-193</sup> |                     | -33.72                                   | 0.2561               |
| O <sub>3</sub>                                 |                                                                    | 4.75 <sup>-183</sup>                               | 0.534               | 38.1 <sup>-183</sup>                     |                      |

**TABLE 5.18** Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*Continued*)

| Substance                            | Viscosity,<br>mN · s · m <sup>-2</sup>                            | Dielectric<br>constant, $\epsilon$                                                                                                                                                                    | Dipole<br>moment, D | Surface tension,<br>mN · m <sup>-1</sup> |                  |
|--------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------|------------------------------------------|------------------|
|                                      |                                                                   |                                                                                                                                                                                                       |                     | <i>a</i>                                 | <i>b</i>         |
| OF <sub>2</sub>                      | 0.662 <sup>9</sup> , 0.529 <sup>25</sup> ,<br>0.439 <sup>50</sup> | 4.096 <sup>34</sup><br>3.9 <sup>20</sup><br>3.43 <sup>25</sup> , 3.50 <sup>17</sup><br>2.85 <sup>160</sup> , 2.7 <sup>165</sup><br>2.813 <sup>-45</sup><br>2.375 <sup>-5</sup><br>2.65 <sup>0.5</sup> | 0.297               | 45.34<br>31.14                           | 0.1283<br>0.1266 |
| O <sub>2</sub> F <sub>2</sub> (FOOF) |                                                                   |                                                                                                                                                                                                       | 1.44                |                                          |                  |
| OsO <sub>4</sub>                     |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| P (lq)                               |                                                                   |                                                                                                                                                                                                       | 0.56                |                                          |                  |
| PBr <sub>3</sub>                     |                                                                   |                                                                                                                                                                                                       | 0.78                |                                          |                  |
| PCl <sub>3</sub>                     |                                                                   |                                                                                                                                                                                                       | 0.9                 |                                          |                  |
| PCl <sub>5</sub>                     |                                                                   |                                                                                                                                                                                                       | 1.03                |                                          |                  |
| PCl <sub>2</sub> F <sub>3</sub>      |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| PCl <sub>3</sub> F <sub>2</sub>      |                                                                   |                                                                                                                                                                                                       | 0.574               |                                          |                  |
| PCl <sub>4</sub> F                   |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| PF <sub>3</sub>                      | 1.065 <sup>25</sup>                                               | 2.9 <sup>15</sup><br>4.12 <sup>65</sup><br>13.7 <sup>25</sup><br>5.8 <sup>22</sup><br>2.78 <sup>20</sup>                                                                                              | 0                   | 61.66                                    | 0.067 71         |
| PF <sub>5</sub>                      |                                                                   |                                                                                                                                                                                                       | 0.574               | 40.44                                    | 0.1158           |
| PH <sub>3</sub>                      |                                                                   |                                                                                                                                                                                                       | 0                   | 35.22                                    | 0.1275           |
| PI <sub>3</sub>                      |                                                                   |                                                                                                                                                                                                       | 2.54                | 37.00                                    | 0.1272           |
| PO <sub>3</sub>                      |                                                                   |                                                                                                                                                                                                       | 1.868               |                                          |                  |
| POCl <sub>3</sub>                    |                                                                   |                                                                                                                                                                                                       | 1.42                |                                          |                  |
| POF <sub>3</sub>                     |                                                                   |                                                                                                                                                                                                       | 0.64                |                                          |                  |
| PSCl <sub>3</sub>                    |                                                                   |                                                                                                                                                                                                       | 57.00               |                                          |                  |
| PSF <sub>3</sub>                     |                                                                   |                                                                                                                                                                                                       | 54.05               |                                          |                  |
| PbCl <sub>4</sub>                    |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| ReO <sub>2</sub> Cl <sub>3</sub>     |                                                                   |                                                                                                                                                                                                       | 0.36                |                                          |                  |
| ReO <sub>3</sub> Cl                  | 0.0153 <sup>27</sup> ,<br>0.0198 <sup>127</sup>                   | 3.499 <sup>134</sup><br>2.915 <sup>25</sup><br>4.79 <sup>15</sup>                                                                                                                                     | 0.36                |                                          |                  |
| S                                    |                                                                   |                                                                                                                                                                                                       | 1.0                 |                                          |                  |
| SCl <sub>2</sub>                     |                                                                   |                                                                                                                                                                                                       | 1.45                | 46.23                                    | 0.1464           |
| S <sub>2</sub> Cl <sub>2</sub> dimer |                                                                   |                                                                                                                                                                                                       | 1.03                |                                          |                  |
| S <sub>2</sub> F <sub>2</sub>        |                                                                   |                                                                                                                                                                                                       | 0.632               |                                          |                  |
| FSSF isomer                          |                                                                   |                                                                                                                                                                                                       | 1.03                |                                          |                  |
| S=SF <sub>2</sub> isomer             |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| SF <sub>4</sub>                      |                                                                   |                                                                                                                                                                                                       | 12.87               |                                          |                  |
| SF <sub>6</sub>                      |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| S <sub>2</sub> F <sub>10</sub>       |                                                                   |                                                                                                                                                                                                       | 5.66                |                                          |                  |
| SO <sub>2</sub> (g)                  | 0.0129 <sup>27</sup> ,<br>0.0175 <sup>127</sup>                   | 2.020 <sup>20</sup><br>1.0093 <sup>0</sup><br>16.3 <sup>25</sup><br>3.11 <sup>18</sup><br>9.06 <sup>20</sup><br>9.25 <sup>20</sup> , 8.675 <sup>25</sup><br>9.15 <sup>20</sup>                        | 0                   |                                          |                  |
| (lq)                                 |                                                                   |                                                                                                                                                                                                       | 1.63                |                                          |                  |
| SO <sub>3</sub>                      |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| SOBr <sub>2</sub>                    |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| SOCl <sub>2</sub>                    |                                                                   |                                                                                                                                                                                                       | 9.11                |                                          |                  |
| SOF <sub>2</sub>                     |                                                                   |                                                                                                                                                                                                       | 1.45                |                                          |                  |
| SO <sub>2</sub> Cl <sub>2</sub>      |                                                                   |                                                                                                                                                                                                       | 1.63                |                                          |                  |
| SO <sub>2</sub> F <sub>2</sub>       |                                                                   |                                                                                                                                                                                                       | 1.81                |                                          |                  |
| SbCl <sub>3</sub>                    |                                                                   |                                                                                                                                                                                                       | 1.12                |                                          |                  |
| SbCl <sub>5</sub>                    |                                                                   |                                                                                                                                                                                                       | 33.2 <sup>75</sup>  |                                          |                  |
| SbF <sub>5</sub>                     | 5.44 <sup>237.5</sup>                                             | 3.22 <sup>20</sup>                                                                                                                                                                                    | 3.93                |                                          |                  |
| SbH <sub>3</sub>                     |                                                                   |                                                                                                                                                                                                       | 0                   |                                          |                  |
| Se (lq)                              |                                                                   |                                                                                                                                                                                                       | 0.12                |                                          |                  |
| SeF <sub>4</sub>                     |                                                                   |                                                                                                                                                                                                       | 1.78                | 49.07                                    | 0.1937           |
|                                      |                                                                   |                                                                                                                                                                                                       |                     | 38.61                                    | 0.1274           |

**TABLE 5.18** Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*Continued*)

| Substance           | Viscosity,<br>$\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ | Dielectric<br>constant, $\epsilon$             | Dipole<br>moment, D | Surface tension,<br>$\text{mN} \cdot \text{m}^{-1}$ |                         |
|---------------------|--------------------------------------------------------------|------------------------------------------------|---------------------|-----------------------------------------------------|-------------------------|
|                     |                                                              |                                                |                     | <i>a</i>                                            | <i>b</i>                |
| SeF <sub>6</sub>    | 99.4 <sup>25</sup> , 96.2 <sup>50</sup>                      | 46.2 <sup>20</sup>                             | 0                   | 20.78                                               | 0.099 62                |
| SeOCl <sub>2</sub>  |                                                              |                                                | 2.64                |                                                     |                         |
| SeO <sub>2</sub>    |                                                              |                                                | 2.62                |                                                     |                         |
| SiCl <sub>4</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| SiF <sub>4</sub>    |                                                              |                                                | 0                   |                                                     |                         |
| SiH <sub>4</sub>    |                                                              | 2.248 <sup>0</sup>                             | 0                   | 20.43                                               | 0.1076                  |
| SiHCl <sub>3</sub>  |                                                              |                                                | 0.86                |                                                     |                         |
| SiH <sub>3</sub> Cl |                                                              |                                                | 1.31                |                                                     |                         |
| SnBr <sub>4</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| SnCl <sub>4</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| TeF <sub>6</sub>    | 0.415 <sup>0</sup> , 0.326 <sup>25</sup>                     | 3.169 <sup>30</sup>                            | 0                   | 29.92                                               | 0.1134                  |
| TiCl <sub>4</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| TiCl <sub>4</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| UF <sub>6</sub> (g) |                                                              |                                                | 0                   |                                                     |                         |
| (lq)                |                                                              |                                                | 0                   |                                                     |                         |
| VCl <sub>4</sub>    |                                                              | 3.014 <sup>0</sup> , 2.89 <sup>20</sup>        | 0                   | 33.54 <sup>20</sup>                                 | 31.06 <sup>40</sup>     |
| VOBr <sub>3</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| VOCl <sub>3</sub>   |                                                              |                                                | 0                   |                                                     |                         |
| Xe (g)              |                                                              |                                                | 0                   |                                                     |                         |
| (lq, ll)            |                                                              |                                                | 0                   |                                                     |                         |
| XeF <sub>6</sub>    |                                                              |                                                | 0                   |                                                     |                         |
|                     | 0.0228 <sup>20</sup> ,<br>0.030 <sup>127</sup>               | 1.880 <sup>-111.9</sup><br>4.10 <sup>125</sup> | 0.3                 | 36.36 <sup>20</sup>                                 | 33.60 <sup>40</sup>     |
|                     |                                                              |                                                |                     |                                                     |                         |
|                     |                                                              |                                                |                     | 0.345 <sup>1.00 K</sup>                             | 0.317 <sup>2.00 K</sup> |

**TABLE 5.19** Refractive Index, Viscosity, Dielectric Constant, and Surface Tension of Water at Various Temperatures

| Temp.,<br>°C | Refractive<br>index, $n_D$ | Viscosity,<br>$\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ | Dielectric<br>constant,<br>$\epsilon$ | Surface<br>tension,<br>$\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ |
|--------------|----------------------------|--------------------------------------------------------------|---------------------------------------|-----------------------------------------------------------------------|
| 0            | 1.333 95                   | 1.793                                                        | 87.90                                 | 75.83                                                                 |
| 5            | 1.333 88                   | 1.521                                                        | 85.84                                 | 75.09                                                                 |
| 10           | 1.333 69                   | 1.307                                                        | 83.96                                 | 74.36                                                                 |
| 15           | 1.333 39                   | 1.135                                                        | 82.00                                 | 73.62                                                                 |
| 20           | 1.333 00                   | 1.002                                                        | 80.20                                 | 72.88                                                                 |
| 25           | 1.332 50                   | 0.890 3                                                      | 78.35                                 | 72.14                                                                 |
| 30           | 1.331 94                   | 0.797 7                                                      | 76.60                                 | 71.40                                                                 |
| 35           | 1.331 31                   | 0.719 0                                                      | 74.83                                 | 70.66                                                                 |
| 40           | 1.330 61                   | 0.653 2                                                      | 73.17                                 | 69.92                                                                 |
| 50           | 1.329 04                   | 0.547 0                                                      | 69.58                                 | 68.45                                                                 |
| 60           | 1.327 25                   | 0.466 5                                                      | 66.73                                 | 66.97                                                                 |
| 70           | 1.325 11                   | 0.404 0                                                      | 63.73                                 | 65.49                                                                 |
| 80           |                            | 0.354 4                                                      | 60.86                                 | 64.01                                                                 |
| 90           |                            | 0.314 5                                                      | 58.12                                 | 62.54                                                                 |
| 100          |                            | 0.281 8                                                      | 55.51                                 | 61.07                                                                 |

### 5.6.1 Refractive Index

The refractive index  $n$  is the ratio of the velocity of light in a particular substance to the velocity of light in vacuum. Values reported refer to the ratio of the velocity in air to that in the substance saturated with air. Usually the yellow sodium doublet lines are used; they have a weighted mean of 589.26 nm and are symbolized by **D**. When only a single refractive index is available, approximate values over a small temperature range may be calculated using a mean value of 0.000 45 per degree for  $dn/dt$ , and remembering that  $n_D$  decreases with an increase in temperature. If a transition point lies within the temperature range, extrapolation is not reliable.

The *specific refraction*  $r_D$  is given by the Lorentz and Lorenz equation,

$$R_D = \frac{n_D^2 - 1}{n_D^2 + 2} \cdot \frac{1}{\rho}$$

where  $\rho$  is the density at the same temperature as the refractive index, and is independent of temperature and pressure. The molar refraction is equal to the specific refraction multiplied by the molecular weight. It is a more or less additive property of the groups or elements comprising the compound. A set of atomic refractions is given in Table 5.19; an extensive discussion will be found in Bauer, Fajans, and Lewin, in *Physical Methods of Organic Chemistry*, 3d ed., A. Weissberger (ed.), vol. 1, part II, chap. 28, Wiley-Interscience, New York, 1960.

The empirical Eykman equation

$$\frac{n_D^2 - 1}{n_D + 0.4} \cdot \frac{1}{\rho} = \text{constant}$$

offers a more accurate means for checking the accuracy of experimental densities and refractive indices, and for calculating one from the other, than does the Lorentz and Lorenz equation.

The refractive index of moist air can be calculated from the expression

$$(n - 1) \times 10^6 = \frac{103.49}{T} p_1 + \frac{177.4}{T} p_2 + \frac{86.26}{T} \left( 1 + \frac{5748}{T} \right) p_3$$

where  $p_1$  is the partial pressure of dry air (in mmHg),  $p_2$  is the partial pressure of carbon dioxide (in mmHg),  $p_3$  is the partial pressure of water vapor (in mmHg), and  $T$  is the temperature (in kelvins).

*Example:* 1-Propynyl acetate has  $n_D = 1.4187$  and density = 0.9982 at 20°C; the molecular weight is 98.102. From the Lorentz and Lorenz equation,

$$r_D = \frac{(1.4187)^2 + 1}{(1.4187)^2 + 2} \cdot \frac{1}{0.9982} = 0.2528$$

The molar refraction is

$$Mr_D = (98.102)(0.2528) = 24.80$$

From the atomic and group refractions in Table 5.19, the molar refraction is computed as follows:

|                |                 |
|----------------|-----------------|
| 6 H            | 6.600           |
| 5 C            | 12.090          |
| 1 C $\equiv$ C | 2.398           |
| 1 O(ether)     | 1.643           |
| 1 O(carbonyl)  | <u>2.211</u>    |
|                | $Mr_D = 24.942$ |

**TABLE 5.20** Atomic and Group Refractions

| Group                                      | $Mr_D$ | Group                             | $Mr_D$ |
|--------------------------------------------|--------|-----------------------------------|--------|
| H                                          | 1.100  | N (primary aliphatic amine)       | 2.322  |
| C                                          | 2.418  | N ( <i>sec</i> -aliphatic amine)  | 2.499  |
| Double bond (C=C)                          | 1.733  | N ( <i>tert</i> -aliphatic amine) | 2.840  |
| Triple bond (C≡C)                          | 2.398  | N (primary aromatic amine)        | 3.21   |
| Phenyl (C <sub>6</sub> H <sub>5</sub> )    | 25.463 | N ( <i>sec</i> -aromatic amine)   | 3.59   |
| Naphthyl (C <sub>10</sub> H <sub>7</sub> ) | 43.00  | N ( <i>tert</i> -aromatic amine)  | 4.36   |
| O (carbonyl) (C=O)                         | 2.211  | N (primary amide)                 | 2.65   |
| O (hydroxyl) (O—H)                         | 1.525  | N ( <i>sec</i> amide)             | 2.27   |
| O (ether, ester) (C—O—)                    | 1.643  | N ( <i>tert</i> amide)            | 2.71   |
| F (one fluoride)                           | 0.95   | N (imidine)                       | 3.776  |
| (polyfluorides)                            | 1.1    | N (oximido)                       | 3.901  |
| Cl                                         | 5.967  | N (carbimido)                     | 4.10   |
| Br                                         | 8.865  | N (hydrazone)                     | 3.46   |
| I                                          | 13.900 | N (hydroxylamine)                 | 2.48   |
| S (thiocarbonyl) (C=S)                     | 7.97   | N (hydrazine)                     | 2.47   |
| S (thiol) (S—H)                            | 7.69   | N (aliphatic cyanide) (C≡N)       | 3.05   |
| S (dithia) (—S—S—)                         | 8.11   | N (aromatic cyanide)              | 3.79   |
| Se (alkyl selenides)                       | 11.17  | N (aliphatic oxime)               | 3.93   |
| 3-membered ring                            | 0.71   | NO (nitroso)                      | 5.91   |
| 4-membered ring                            | 0.48   | NO (nitrosoamine)                 | 5.37   |
|                                            |        | NO <sub>2</sub> (alkyl nitrate)   | 7.59   |
|                                            |        | (alkyl nitrite)                   | 7.44   |
|                                            |        | (aliphatic nitro)                 | 6.72   |
|                                            |        | (aromatic nitro)                  | 7.30   |
|                                            |        | (nitramine)                       | 7.51   |

### 5.6.2 Surface Tension

The surface tension of a liquid,  $\gamma$ , is the force per unit length on the surface that opposes the expansion of the surface area. In the literature the surface tensions are expressed in  $\text{dyn} \cdot \text{cm}^{-1}$ ;  $1 \text{ dyn} \cdot \text{cm}^{-1} = 1 \text{ mN} \cdot \text{m}^{-1}$  in the SI system. For the large majority of compounds the dependence of the surface tension on the temperature can be given as

$$\gamma = a - bt$$

where  $a$  and  $b$  are constants and  $t$  is the temperature in degrees Celsius. The values of  $a$  and  $b$  given in Tables 5.16 and 5.18 can be used to calculate the values of surface tension for the particular compound within its liquid range. For example, the least-squares constants for acetic anhydride (liquid from  $-73$  to  $140^\circ\text{C}$ ) are 35.52 and 0.1436, respectively. At  $20^\circ\text{C}$ ,  $\gamma = 35.52 - 0.1436(20) = 32.64 \text{ dyn} \cdot \text{cm}^{-1}$ .

A compilation of data of some 2200 pure liquid compounds has been prepared by Jasper, *J. Phys. Chem. Reference Data* **1**:841 (1972).

### 5.6.3 Dipole Moments

The permanent dipole moment of an isolated molecule depends on the magnitude of the charge and on the distance separating the positive and negative charges. It is defined as

$$\mu = \left( \sum_i q_i r_i \right)$$

where the summation extends over all charges (electrons and nuclei) in the molecule. The numerical values of the dipole moment, expressed in the c.g.s. system of units, are in debye units, D, where  $1 \text{ D} = 10^{-18} \text{ esu of charge} \times \text{centimeters}$ . The conversion factor to SI units is

$$1 \text{ D} = 3.335\,64 \times 10^{-30} \text{ C} \cdot \text{m} \quad [\text{coulomb-meter}]$$

Tables 5.17 and 5.18 contain a selected group of compounds for which the dipole moment is given. An extensive collection of dipole moments (approximately 7000 entries) is contained in A. L. McClellan, *Tables of Experimental Dipole Moments*, W. H. Freeman, San Francisco, 1963. A critical survey of 500 compounds in the gas phase is given by Nelson, Lide, and Maryott, NSRDS-NBS 10, Washington, D.C., 1967.

### 5.6.4 Dielectric Constants

If two oppositely charged plates exist in a vacuum, there is a certain force of attraction between them, as stated by Coulomb's law:

$$F = \frac{1}{4\pi\epsilon_0} \cdot \frac{q_1 q_2}{\epsilon r^2}$$

where  $F$  is the force, in newtons, acting on each of the charges  $q_1$  and  $q_2$ ,  $r$  is the distance between the charges,  $\epsilon$  is the dielectric constant of the medium between the plates, and  $\epsilon_0$  is the permittivity of free space.  $q_1$ ,  $q_2$  are expressed in coulombs and  $r$  in meters. If another substance, such as a solvent, is in the space separating these charges (or ions in a solution), their attraction for each other is less. The dielectric constant is a measure of the relative effect a solvent has on the force with which two oppositely charged plates attract each other. The dielectric constant is a unitless number.

Dielectric constants for a selected group of inorganic and organic compounds are included in Tables 5.17 and 5.18. An extensive list has been compiled by Maryott and Smith, *National Bureau Standards Circular 514*, Washington, D.C., 1951.

For gases the values of the dielectric constant can be adjusted to somewhat different conditions of temperature and pressure by means of the equation

$$\frac{(\epsilon - 1)_{t,p}}{(\epsilon - 1)_{20^\circ, 1 \text{ atm}}} = \frac{p}{760[1 + 0.003\,411(t - 20)]}$$

where  $p$  is the pressure (in mmHg) and  $t$  is the temperature (in  $^\circ\text{C}$ ). The errors associated with this equation probably do not exceed 0.02% for gases between 10 and  $30^\circ\text{C}$  and for pressures between 700 and 800 mm. The dielectric constants of selected gases will be found in Table. 5.18.

### 5.6.5 Viscosity

The *dynamic viscosity*, or coefficient of viscosity,  $\eta$  of a Newtonian fluid is defined as the force per unit area necessary to maintain a unit velocity gradient at right angles to the direction of flow between two parallel planes a unit distance apart. The SI unit is pascal-second or newton-second per meter squared [ $\text{N} \cdot \text{s} \cdot \text{m}^{-2}$ ]. The c.g.s. unit of viscosity is the poise [P];  $1 \text{ cP} \equiv 1 \text{ mN} \cdot \text{s} \cdot \text{m}^{-2}$ . The dynamic viscosity decreases with the temperature approximately according to the equation:  $\log \eta = A + B/T$ . Values of  $A$  and  $B$  for a large number of liquids are given by Barrer, *Trans. Faraday Soc.* **39:48** (1943).

TABLE 5.21 Aqueous Glycerol Solutions

| % Weight glycerol | Grams per liter | Relative density 25°/25°C | Viscosity, mN · s · m <sup>-2</sup> |       |       |
|-------------------|-----------------|---------------------------|-------------------------------------|-------|-------|
|                   |                 |                           | 20°C                                | 25°C  | 30°C  |
| 100               | 1261            | 1.262 01                  | 1 495                               | 942   | 622   |
| 99                | 1246            | 1.259 45                  | 1 194                               | 772   | 509   |
| 98                | 1231            | 1.256 85                  | 971                                 | 627   | 423   |
| 97                | 1216            | 1.254 25                  | 802                                 | 521   | 353   |
| 96                | 1201            | 1.251 65                  | 659                                 | 434   | 296   |
| 95                | 1186            | 1.249 10                  | 543.5                               | 365   | 248   |
| 80                | 966.8           | 1.209 25                  | 61.8                                | 45.72 | 34.81 |
| 50                | 563.2           | 1.127 20                  | 6.032                               | 5.024 | 4.233 |
| 25                | 265.0           | 1.061 15                  | 2.089                               | 1.805 | 1.586 |
| 10                | 102.2           | 1.023 70                  | 1.307                               | 1.149 | 1.021 |

*Kinematic viscosity*  $\nu$  is the ratio of the dynamic viscosity to the density of a fluid. The SI unit is meter squared per second [m<sup>2</sup> · s<sup>-1</sup>]. The c.g.s. units are called stokes [cm<sup>2</sup> · s<sup>-1</sup>]; poises = stokes × density.

*Fluidity*  $\phi$  is the reciprocal of the dynamic viscosity.

The primary reference liquid for viscosity measurements is water. The absolute viscosity of water at 20°C is 1.0019 (±0.0003) mN · s · m<sup>-2</sup> (or centipoise), as determined by Swindells, Coe, and Godfrey, *J. Research Natl. Bur. Standards* **48**:1 (1952). The relative viscosity of water,  $\eta/\eta_{20^\circ}$ , is 0.8885 at 25°C, 0.7960 at 30°C, and 0.6518 at 40°C. Values at temperatures between 15 and 60°C are best represented by Cragoe’s equation:

$$\log \frac{\eta}{\eta_{20^\circ}} = \frac{1.2348(20 - t) - 0.001\,467(t - 20)^2}{t + 96}$$

The *Reynolds number* for flow in a tube is defined by  $d\bar{v}\rho/\eta$ , where  $d$  is the diameter of the tube,  $\bar{v}$  is the average velocity of the fluid along the tube,  $\rho$  is the density of the fluid, and  $\eta$  is its dynamic viscosity. At flow velocities corresponding with values of the Reynolds number of greater than 2000, turbulence is encountered.

TABLE 5.22 Aqueous Sucrose Solutions

| % Weight sucrose | Grams per liter | Relative density 20°/4°C | Viscosity, mN · s · m <sup>-2</sup> |       |       |
|------------------|-----------------|--------------------------|-------------------------------------|-------|-------|
|                  |                 |                          | 15°C                                | 20°C  | 25°C  |
| 75               | 1034            | 1.379 0                  | 4 039                               | 2 328 | 1 405 |
| 70               | 943.0           | 1.347 2                  | 746.9                               | 481.6 | 321.6 |
| 65               | 855.6           | 1.316 3                  | 211.3                               | 147.2 | 105.4 |
| 60               | 771.9           | 1.286 5                  | 79.49                               | 58.49 | 40.03 |
| 50               | 614.8           | 1.299 6                  | 19.53                               | 15.43 | 12.40 |
| 40               | 470.6           | 1.176 4                  | 7.463                               | 6.167 | 5.164 |
| 30               | 338.1           | 1.127 0                  | 3.757                               | 3.187 | 2.735 |

5.7 COMBUSTIBLE MIXTURES

TABLE 5.23 Properties of Combustible Mixtures in Air

The *autoignition temperature* is the minimum temperature required for self-sustained combustion in the absence of an external ignition source. The value depends on specified test conditions. The *flammable (explosive) limits* specify the range of concentration of the vapor in air (in percent by volume) for which a flame can propagate. Below the lower flammable limit, the gas mixture is too lean to burn; above the flammable limit, the mixture is too rich. Additional compounds can be found in National Fire Protection Association, National Fire Protection Handbook, 14th ed., 1991.

For alternative nomenclature, see Table 1.15.

| Substance                       | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|---------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                 |                                 | Lower                                                                           | Upper |
| Acetaldehyde                    | 175                             | 4.0                                                                             | 60    |
| Acetanilide                     | 540                             |                                                                                 |       |
| Acetic acid, glacial            | 463                             | 4.0                                                                             | 19.9  |
| Acetic anhydride                | 316                             | 2.7                                                                             | 10.3  |
| Acetone                         | 465                             | 2.5                                                                             | 12.8  |
| Acetonitrile                    | 524                             | 3.0                                                                             | 16.0  |
| Acetophenone                    | 570                             |                                                                                 |       |
| Acetylacetone                   | 340                             |                                                                                 |       |
| Acetylene                       | 305                             | 3.0                                                                             | 65    |
| Acetyl chloride                 | 390                             |                                                                                 |       |
| Acrolein                        | 220                             | 2.8                                                                             | 31.0  |
| Acrylic acid (2-propenoic acid) | 438                             | 2.4                                                                             | 8.0   |
| Acrylonitrile                   | 481                             | 3.0                                                                             | 17.0  |
| Adiponitrile                    | 550                             | 2                                                                               | 5     |
| Allyl acetate                   | 374                             |                                                                                 |       |
| Allyl alcohol                   | 378                             | 2.5                                                                             | 18.0  |
| Allylamine                      | 374                             | 2.2                                                                             | 22    |
| Ammonia, anhydrous              | 651                             | 16                                                                              | 25    |
| Aniline                         | 615                             | 1.3                                                                             | 11    |
| Asphalt                         | 485                             |                                                                                 |       |
| Benzaldehyde                    | 192                             |                                                                                 |       |
| Benzene                         | 498                             | 1.2                                                                             | 7.8   |
| Benzoyl peroxide                | 80                              |                                                                                 |       |
| Benzyl acetate                  | 460                             |                                                                                 |       |
| Benzyl alcohol                  | 436                             |                                                                                 |       |
| Benzyl benzoate                 | 480                             |                                                                                 |       |
| Benzyl chloride                 | 585                             | 1.1                                                                             |       |
| Bis(2-aminoethyl)amine          | 399                             |                                                                                 |       |
| Bis(2-chloroethyl) ether        | 369                             | 2.7                                                                             |       |
| Biscyclohexyl                   | 245                             | 0.7                                                                             | 5.1   |
| Bis(2-hydroethyl) ether         | 229                             |                                                                                 |       |
| Bromobenzene                    | 565                             |                                                                                 |       |
| 1-Bromobutane                   | 265                             | 2.6                                                                             | 6.6   |
| Bromoethane                     | 511                             | 6.8                                                                             | 8.0   |
| Bromomethane                    | 537                             | 10                                                                              | 16.0  |
| 1-Bromopropane                  | 490                             |                                                                                 |       |



**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                                | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|------------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                          |                                 | Lower                                                                           | Upper |
| 3-Bromopropene                           | 295                             | 4.4                                                                             | 7.3   |
| 1,3-Butadiene                            | 420                             | 2.0                                                                             | 11.5  |
| Butanal (butyraldehyde)                  | 218                             | 1.9                                                                             | 12.5  |
| Butane                                   | 287                             | 1.9                                                                             | 8.5   |
| 1,3-Butanediol                           | 395                             |                                                                                 |       |
| 2,3-Butanediol                           | 402                             |                                                                                 |       |
| Butanenitrile                            | 501                             | 1.65                                                                            |       |
| Butanoic acid (butyric acid)             | 443                             | 2.0                                                                             | 10.0  |
| Butanoic anhydride (butyric anhydride)   | 279                             | 0.9                                                                             | 5.8   |
| 1-Butanol                                | 343                             | 1.4                                                                             | 11.2  |
| 2-Butanol                                | 415                             | 1.7                                                                             | 11    |
| 2-Butanone                               | 404                             | 1.4                                                                             | 11.4  |
| <i>trans</i> -2-Butenal (crotonaldehyde) | 232                             | 2.1                                                                             | 15.9  |
| 1-Butene                                 | 384                             | 1.6                                                                             | 9.3   |
| <i>cis</i> -2-Butene                     | 324                             | 1.7                                                                             |       |
| <i>trans</i> -2-Butene                   | 324                             | 1.8                                                                             | 9.7   |
| 1-Butene oxide                           |                                 | 1.5                                                                             | 18.3  |
| 3-Buten-1-ol                             |                                 | 4.7                                                                             | 34    |
| 2-Butoxyethanol                          | 238                             | 4                                                                               | 13    |
| 2-(2-Butoxyethoxy)ethyl acetate          | 299                             |                                                                                 |       |
| Butyl acetate                            | 425                             | 1.7                                                                             | 7.6   |
| <i>sec</i> -Butyl acetate                |                                 | 1.7                                                                             | 9.8   |
| Butylamine                               | 312                             | 1.7                                                                             | 9.8   |
| <i>tert</i> -Butylamine                  | 380                             | 1.7                                                                             | 8.9   |
| Butylbenzene                             | 410                             | 0.8                                                                             | 5.8   |
| <i>sec</i> -Butylbenzene                 | 418                             | 0.8                                                                             | 6.9   |
| <i>tert</i> -Butylbenzene                | 450                             | 0.7                                                                             | 5.7   |
| Butyl formate                            | 322                             | 1.7                                                                             | 8.2   |
| Butyl methyl ketone                      | 423                             | 1                                                                               | 8     |
| Butyl 2-methyl-2-propenoate              | 294                             | 2                                                                               | 8     |
| Butyl propanoate                         | 427                             |                                                                                 |       |
| Butyl stearate                           | 355                             |                                                                                 |       |
| Butyl vinyl ether                        | 255                             |                                                                                 |       |
| 2-Butyne                                 |                                 | 1.4                                                                             |       |
| Camphor                                  | 466                             | 0.6                                                                             | 3.5   |
| Carbon disulfide                         | 90                              | 1.3                                                                             | 50.0  |
| Carbon monoxide                          | 609                             | 12.5                                                                            | 74.2  |
| Carbonyl sulfide                         |                                 | 12                                                                              | 28.5  |
| Chlorobenzene                            | 593                             | 1.3                                                                             | 9.6   |
| 1-Chloro-1,3-butadiene                   |                                 | 4.0                                                                             | 20.0  |
| 1-Chlorobutane                           | 240                             | 1.8                                                                             | 10.1  |
| 2-Chloro-2-butene                        |                                 | 2.3                                                                             | 9.3   |
| 1-Chloro-2,3-epoxypropane                | 411                             | 4                                                                               | 21    |
| 1-Chloro-1,1-difluoroethane              |                                 | 6.2                                                                             | 17.9  |
| 1-Chloro-2,4-dinitrobenzene              |                                 | 2.0                                                                             | 22    |
| 1-Chloro-2,3-epoxypropane                | 411                             | 3.8                                                                             | 21    |
| Chloroethane                             | 519                             | 3.8                                                                             | 15.4  |
| 2-Chloroethanol                          | 425                             | 4.9                                                                             | 15.9  |
| Chloromethane                            | 632                             | 8.1                                                                             | 17.4  |
| 1-Chloro-3-methylbutane                  |                                 | 1.5                                                                             | 7.4   |
| 1-Chloro-2-methylpropane                 |                                 | 2.0                                                                             | 8.8   |

**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                                     | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|-----------------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                               |                                 | Lower                                                                           | Upper |
| 3-Chloro-2-methyl-1-propene                   |                                 | 2.3                                                                             | 9.3   |
| 1-Chloronaphthalene                           | >588                            |                                                                                 |       |
| 1-Chloropentane                               | 260                             | 1.6                                                                             | 8.6   |
| 1-Chloropropane                               | 520                             | 2.6                                                                             | 11.1  |
| 2-Chloropropane                               | 593                             | 2.8                                                                             | 10.7  |
| 1-Chloro-1-propene                            |                                 | 4.5                                                                             | 16    |
| 2-Chloro-1-propene                            |                                 | 4.5                                                                             | 16    |
| 3-Chloro-1-propene                            | 485                             | 2.9                                                                             | 11.1  |
| Chlorotrifluoroethylene                       |                                 | 24                                                                              | 40.3  |
| <i>m</i> -Cresol                              | 558                             | 1.1                                                                             |       |
| <i>o</i> -Cresol                              | 599                             | 1.4                                                                             |       |
| <i>p</i> -Cresol                              | 558                             | 1.1                                                                             |       |
| Cumene                                        | 424                             | 0.9                                                                             | 6.5   |
| Cyanogen                                      |                                 | 6.6                                                                             | 32    |
| Cyclobutane                                   |                                 | 1.8                                                                             |       |
| Cyclohexane                                   | 245                             | 1.3                                                                             | 8     |
| Cyclohexanol                                  | 300                             | 1                                                                               | 9     |
| Cyclohexanone                                 | 420                             | 1.1                                                                             | 9.4   |
| Cyclohexene                                   | 244                             | 1.2                                                                             |       |
| Cyclohexyl acetate                            | 334                             |                                                                                 |       |
| Cyclohexylamine                               | 293                             | 1                                                                               | 9     |
| Cyclopentane                                  | 361                             | 1.5                                                                             |       |
| Cyclopentene                                  | 395                             |                                                                                 |       |
| Cyclopropane                                  | 500                             | 2.4                                                                             | 10.4  |
| <i>p</i> -Cymene                              | 436                             | 0.7                                                                             | 5.6   |
| <i>trans</i> -Decahydronaphthalene            | 255                             | 0.7                                                                             | 5.4   |
| Decane                                        | 210                             | 0.8                                                                             | 5.4   |
| Decene                                        | 235                             |                                                                                 |       |
| Diborane(6)                                   | 38 to 52                        | 0.8                                                                             | 88    |
| Dibutylamine                                  |                                 | 1.1                                                                             | 6     |
| Dibutyl decanedioate (dibutyl sebacate)       | 365                             | 0.44                                                                            |       |
| Dibutyl ether                                 | 194                             | 1.5                                                                             | 7.6   |
| Dibutyl <i>o</i> -phthalate                   | 402                             | 0.5                                                                             |       |
| 1,2-Dichlorobenzene                           | 648                             | 2.2                                                                             | 9.2   |
| 1,1-Dichloroethane                            | 458                             | 5.4                                                                             | 11.4  |
| 1,2-Dichloroethane                            | 413                             | 6.2                                                                             | 16    |
| 1,1-Dichloroethylene                          | 570                             | 6.5                                                                             | 15.5  |
| <i>cis</i> -1,2-Dichloroethylene              | 460                             | 3                                                                               | 15    |
| <i>trans</i> -1,2-Dichloroethylene            | 460                             | 6                                                                               | 13    |
| Dichloromethane                               | 556                             | 13                                                                              | 23    |
| 1,2-Dichloropropane                           | 557                             | 3.4                                                                             | 14.5  |
| Diethanolamine [2,2'-iminobis(ethanol)]       | 662                             | 2                                                                               | 13    |
| 1,1-Diethoxyethane (acetal)                   | 230                             | 1.6                                                                             | 10.4  |
| Diethylamine                                  | 312                             | 1.8                                                                             | 10.1  |
| Diethylene glycol [bis(2-hydroxyethyl) ether] | 224                             | 2                                                                               | 17    |
| Diethylene glycol dibutyl ether               | 310                             |                                                                                 |       |
| Diethylene glycol monoethyl ether acetate     | 425                             |                                                                                 |       |
| Diethylene glycol monomethyl ether            | 240                             | 1.4                                                                             | 22.7  |
| Diethylenetriamine                            | 358                             | 2                                                                               | 6.7   |
| Diethyl ether                                 | 180                             | 1.9                                                                             | 36.0  |
| 3,3-Diethylpentane                            | 290                             | 0.7                                                                             | 5.7   |

**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                             | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|---------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                       |                                 | Lower                                                                           | Upper |
| Diethyl peroxide                      |                                 | 2.3                                                                             | 15.9  |
| Diethyl sulfate                       | 436                             |                                                                                 |       |
| 1,1-Difluoroethylene                  |                                 | 5.5                                                                             | 21.3  |
| 1,3-Dihydroxybenzene (resorcinol)     | 664                             |                                                                                 |       |
| 1,4-Dihydroxybenzene                  | 516                             |                                                                                 |       |
| Diisopropylamine                      | 316                             | 1.1                                                                             | 7.1   |
| Diisopropyl ether                     | 443                             | 1.4                                                                             | 7.9   |
| Dimethoxymethane                      | 237                             | 2.2                                                                             | 13.8  |
| <i>N,N</i> -Dimethylacetamide         | 490                             | 2.0                                                                             | 11.5  |
| Dimethylamine (anhydrous)             | 400                             | 2.8                                                                             | 14.4  |
| <i>N,N</i> -Dimethylaniline           | 371                             |                                                                                 |       |
| 2,3-Dimethylaniline                   |                                 | 1.0                                                                             |       |
| 2,2-Dimethylbutane                    | 405                             | 1.2                                                                             | 7.0   |
| 2,3-Dimethylbutane                    | 405                             | 1.2                                                                             | 7.0   |
| 3,3-Dimethyl-2-butanone               | 423                             | 1                                                                               | 8     |
| <i>cis</i> -1,2-Dimethylcyclohexane   | 304                             |                                                                                 |       |
| <i>trans</i> -1,2-Dimethylcyclohexane | 304                             |                                                                                 |       |
| Dimethyl ether                        | 350                             | 3.4                                                                             | 27.0  |
| <i>N,N</i> -Dimethylformamide         | 445                             | 2.2                                                                             | 15.2  |
| 2,6-Dimethyl-4-heptanol               |                                 | 0.8                                                                             | 6.1   |
| 2,6-Dimethyl-4-heptanone              | 396                             | 0.8                                                                             | 6.2   |
| 2,3-Dimethylhexane                    | 438                             |                                                                                 |       |
| 1,1-Dimethylhydrazine                 | 249                             | 2                                                                               | 95    |
| 2,3-Dimethylpentane                   | 335                             | 1.1                                                                             | 6.7   |
| Dimethyl 1,2-phthalate                | 490                             | 0.9                                                                             |       |
| 2,2-Dimethylpropane                   | 450                             | 1.4                                                                             | 7.5   |
| Dimethyl sulfate                      | 188                             |                                                                                 |       |
| Dimethyl sulfide                      | 206                             | 2.2                                                                             | 19.7  |
| Dimethyl sulfoxide                    | 215                             | 2.6                                                                             | 42    |
| 1,4-Dioxane                           | 180                             | 2.0                                                                             | 22    |
| Dipentene                             | 237                             |                                                                                 |       |
| Dipentyl ether                        | 170                             |                                                                                 |       |
| Diphenylamine                         | 634                             |                                                                                 |       |
| Diphenyl ether                        | 618                             | 0.8                                                                             | 1.5   |
| Dipropylamine                         | 299                             |                                                                                 |       |
| Dipropyl ether                        | 188                             | 1.3                                                                             | 7.0   |
| Divinyl ether                         | 360                             | 1.7                                                                             | 27.0  |
| Dodecane                              | 203                             | 0.6                                                                             |       |
| 1-Dodecanol                           | 275                             |                                                                                 |       |
| 1,2-Epoxybutane                       | 439                             | 1.7                                                                             | 19    |
| Ethane                                | 515                             | 3.0                                                                             | 12.5  |
| 1,2-Ethanediamine                     | 385                             | 2.5                                                                             | 12.0  |
| 1,2-Ethanediol                        | 398                             | 3.2                                                                             | 22    |
| Ethanethiol                           | 299                             | 2.8                                                                             | 18.2  |
| Ethanol                               | 363                             | 3.3                                                                             | 19    |
| Ethanolamine                          | 410                             | 3.0                                                                             | 23.5  |
| 2-Ethoxyethanol                       | 235                             | 3                                                                               | 18    |
| 2-Ethoxyethyl acetate                 | 379                             | 2                                                                               | 8     |
| 1-Ethoxypropane                       |                                 | 1.7                                                                             | 9.0   |
| Ethyl acetate                         | 426                             | 2                                                                               | 11.5  |
| Ethyl acetoacetate                    | 295                             | 1.4                                                                             | 9.5   |

**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                            | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|--------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                      |                                 | Lower                                                                           | Upper |
| Ethyl acrylate                       | 372                             | 1.4                                                                             | 14    |
| Ethylamine                           | 385                             | 3.5                                                                             | 14.0  |
| Ethylbenzene                         | 432                             | 0.8                                                                             | 6.7   |
| Ethyl benzoate                       | 490                             |                                                                                 |       |
| Ethyl butanoate                      | 463                             |                                                                                 |       |
| 2-Ethylbutanoic acid                 | 463                             |                                                                                 |       |
| Ethyl chloroformate                  | 500                             |                                                                                 |       |
| Ethylcyclobutane                     | 210                             | 1.2                                                                             | 7.7   |
| Ethylcyclohexane                     | 238                             | 0.9                                                                             | 6.6   |
| Ethylene                             | 490                             | 2.7                                                                             | 36.0  |
| Ethylene glycol diacetate            | 482                             | 1.6                                                                             | 8.4   |
| Ethylene glycol dimethyl ether       | 202                             |                                                                                 |       |
| Ethylene glycol ethyl ether acetate  | 379                             | 2                                                                               | 8     |
| Ethylene glycol monobutyl ether      | 238                             | 4                                                                               | 13    |
| Ethylene glycol methyl ether acetate | 392                             | 2                                                                               | 12    |
| Ethylene glycol monoethyl ether      | 235                             | 3                                                                               | 18    |
| Ethyleneimine                        | 320                             | 3.3                                                                             | 54.8  |
| Ethylene oxide                       | 429                             | 3.0                                                                             | 100   |
| Ethyl formate                        | 455                             | 2.8                                                                             | 16.0  |
| 2-Ethylhexanal                       | 197                             |                                                                                 |       |
| 2-Ethyl-1,3-hexanediol               | 360                             |                                                                                 |       |
| 2-Ethyl-1-hexanol                    | 231                             | 0.88                                                                            | 9.7   |
| 2-Ethylhexyl acetate                 | 268                             | 0.76                                                                            | 8.14  |
| Ethyl lactate                        | 400                             | 1.5                                                                             |       |
| Ethyl methyl ether                   |                                 | 2.0                                                                             | 10.0  |
| 3-Ethyl-2-methylpentane              | 460                             |                                                                                 |       |
| Ethyl nitrate                        | 85 explodes                     | 3.8                                                                             |       |
| Ethyl nitrite                        | 90 explodes                     | 3.0                                                                             | 50.0  |
| Ethyl propanoate                     | 440                             | 1.9                                                                             | 11    |
| Ethyl vinyl ether                    | 202                             | 1.7                                                                             | 28    |
| Formaldehyde                         | 430                             | 7.0                                                                             | 73.0  |
| Formic acid, 90%                     | 434                             | 18                                                                              | 57    |
| 2-Furaldehyde (furfural)             | 316                             | 2.1                                                                             | 19.3  |
| Furan                                |                                 | 2.3                                                                             | 14.3  |
| Furfuryl alcohol                     | 491                             | 1.8                                                                             | 16.3  |
| Gasoline, 50-100 octane              | 280 to 456                      | 1.4                                                                             | 7.6   |
| Glycerol                             | 370                             | 3                                                                               | 19    |
| Heptane                              | 204                             | 1.05                                                                            | 6.7   |
| 2-Heptanone (methyl pentyl ketone)   | 393                             | 1.1                                                                             | 7.9   |
| 4-Heptanone (diisobutyl ketone)      | 396                             | 0.8                                                                             | 7.1   |
| 1-Heptene                            | 260                             |                                                                                 |       |
| 1,1,2,3,4,4-Hexachlorobutadiene      | 610                             |                                                                                 |       |
| Hexane                               | 225                             | 1.1                                                                             | 7.5   |
| 1,6-Hexanedioic acid                 | 420                             |                                                                                 |       |
| Hexanoic acid                        | 380                             |                                                                                 |       |
| 2-Hexanone                           | 423                             | 1                                                                               | 8     |
| 1-Hexene                             | 253                             |                                                                                 |       |
| Hydrazine                            | 23 to 270                       | 4.7                                                                             | 100   |
| Hydrogen                             | 400                             | 4.1                                                                             | 74.2  |
| Hydrogen cyanide, 96%                | 538                             | 5.6                                                                             | 40.0  |
| Hydrogen sulfide                     | 260                             | 4                                                                               | 46    |

TABLE 5.23 Properties of Combustible Mixtures in Air (Continued)

| Substance                                        | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|--------------------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                                  |                                 | Lower                                                                           | Upper |
| N-Hydroxyethyl-1,2-ethanediamine                 | 368                             |                                                                                 |       |
| 1-Hydroxy-2-methylbenzene                        | 599                             | 1.4                                                                             |       |
| 1-Hydroxy-3-methylbenzene                        | 559                             | 1.1                                                                             |       |
| 1-Hydroxy-4-methylbenzene (see <i>p</i> -cresol) |                                 |                                                                                 |       |
| 4-Hydroxy-4-methyl-2-pentanone                   | 643                             | 1.8                                                                             | 6.9   |
| Isobutanal                                       | 196                             | 1.6                                                                             | 10.6  |
| Isobutyl acetate                                 | 421                             | 1                                                                               | 10.5  |
| Isobutylamine                                    | 378                             | 2                                                                               | 12    |
| Isobutylbenzene                                  | 427                             | 0.8                                                                             | 6.0   |
| Isobutyl isobutyrate                             | 432                             | 0.96                                                                            | 7.59  |
| Isopentane                                       | 420                             | 1.4                                                                             | 7.6   |
| Isopentyl acetate                                | 360                             | 1.0                                                                             | 7.5   |
| Isoprene                                         | 220                             | 2                                                                               | 9     |
| Isopropyl acetate                                | 460                             | 1.8                                                                             | 8     |
| Isopropyl alcohol                                | 399                             | 2.5                                                                             | 12.7  |
| Isopropylamine                                   | 402                             | 2.3                                                                             | 10.4  |
| Isopropylbenzene (cumene)                        | 424                             | 0.8                                                                             | 6.5   |
| Isopropyl formate                                | 485                             |                                                                                 |       |
| 4-Isopropyl-1-methylbenzene                      | 436                             |                                                                                 |       |
| Kerosene                                         | 210                             | 0.7                                                                             | 5.0   |
| Maleic anhydride                                 | 477                             | 1.4                                                                             | 7.1   |
| Methacrylic acid                                 | 68                              | 1.6                                                                             | 8.8   |
| Methacrylonitrile                                |                                 | 2                                                                               | 6.8   |
| Methane                                          | 650                             | 5.3                                                                             | 15.0  |
| Methanethiol                                     |                                 | 3.9                                                                             | 21.8  |
| Methanol                                         | 464                             | 6.0                                                                             | 36    |
| Methoxybenzene (anisole)                         | 475                             |                                                                                 |       |
| 2-Methoxyethanol                                 | 285                             | 1.8                                                                             | 14    |
| 2-Methoxyethyl acetate                           | 392                             | 1.5                                                                             | 12.3  |
| Methyl acetate                                   | 454                             | 3.1                                                                             | 16    |
| Methyl acetoacetate                              | 280                             |                                                                                 |       |
| Methyl acetylacetate                             | 280                             |                                                                                 |       |
| Methyl acrylate                                  | 468                             | 2.8                                                                             | 25    |
| Methylamine                                      | 430                             | 4.9                                                                             | 20.7  |
| 2-Methylbutane                                   |                                 | 1.4                                                                             | 7.6   |
| 2-Methyl-1-butanol                               | 385                             | 1.4                                                                             | 9.0   |
| 2-Methyl-2-butanol                               | 437                             | 1.2                                                                             | 9.0   |
| 3-Methyl-1-butanol                               | 350                             | 1.2                                                                             | 9.0   |
| 3-Methylbutyl acetate                            | 360                             | 1.0                                                                             | 7.5   |
| 2-Methyl-2-butene                                | 275                             | 1.6                                                                             | 8.7   |
| 3-Methyl-1-butene                                | 365                             | 1.5                                                                             | 9.1   |
| 2-Methyl-1-buten-3-one                           |                                 | 1.8                                                                             | 9.0   |
| Methyl chloroformate                             | 504                             |                                                                                 |       |
| Methylcyclohexane                                | 250                             | 1.2                                                                             | 6.7   |
| cis-2-Methylcyclohexanol                         | 296                             |                                                                                 |       |
| trans-2-Methylcyclohexanol                       | 296                             |                                                                                 |       |
| cis-4-Methylcyclohexanol                         | 295                             |                                                                                 |       |
| trans-4-Methylcyclohexanol                       | 295                             |                                                                                 |       |
| Methylcyclopentane                               | 258                             | 1.0                                                                             | 8.35  |
| Methyl formate                                   | 449                             | 4.5                                                                             | 23    |
| 2-Methylhexane                                   | 280                             | 1.0                                                                             | 6.0   |

**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                                            | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|------------------------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                                      |                                 | Lower                                                                           | Upper |
| 3-Methylhexane                                       | 280                             |                                                                                 |       |
| 5-Methyl-2-hexanone                                  | 191                             | 1.0                                                                             | 8.2   |
| Methylhydrazine                                      | 196                             | 2.5                                                                             | 97.±2 |
| Methyl isobutyl ketone (MIBK)                        | 448                             | 1                                                                               | 8     |
| 2-Methylacetonitrile                                 | 688                             |                                                                                 |       |
| Methyl methacrylate                                  |                                 | 1.7                                                                             | 8.2   |
| 1-Methyl-4-(1-methylethenyl)-cyclohexene (dipentene) | 237                             |                                                                                 |       |
| 1-Methylnaphthalene                                  | 529                             |                                                                                 |       |
| 2-Methylpentane                                      | 264                             | 1.0                                                                             | 7.0   |
| 3-Methylpentane                                      | 278                             | 1.2                                                                             | 7.0   |
| 2-Methyl-2,4-pentanediol                             | 306                             | 1                                                                               | 9     |
| 2-Methyl-1-pentanol                                  | 310                             | 1.1                                                                             | 9.65  |
| 4-Methyl-2-pentanol                                  |                                 | 1.0                                                                             | 5.5   |
| 4-Methyl-2-pentanone                                 | 452                             | 2                                                                               | 8.0   |
| 4-Methyl-3-penten-2-one                              | 344                             | 1.4                                                                             | 7.2   |
| 2-Methylpropanal                                     | 223                             | 1.6                                                                             | 10.6  |
| 2-Methyl-1-propanamine                               | 378                             | 2                                                                               | 12    |
| 2-Methylpropane                                      | 460                             | 1.8                                                                             | 8.4   |
| 2-Methylpropanenitrile                               | 482                             |                                                                                 |       |
| Methyl propanoate                                    | 469                             | 2.5                                                                             | 13    |
| 2-Methylpropanoic acid                               | 481                             | 2.0                                                                             | 9.2   |
| 2-Methyl-1-propanol                                  | 415                             | 1.7                                                                             | 10.6  |
| 2-Methyl-2-propanol ( <i>t</i> -butyl alcohol)       | 478                             | 2.4                                                                             | 8.0   |
| 2-Methyl-1-propene                                   | 465                             | 1.8                                                                             | 9.6   |
| 2-Methylpropyl acetate                               | 421                             | 1.3                                                                             | 10.5  |
| 2-Methylpropyl formate                               | 320                             | 1.7                                                                             | 8     |
| 2-Methylpyridine                                     | 538                             |                                                                                 |       |
| <i>N</i> -Methyl-2-pyrrolidone                       | 346                             | 1                                                                               | 10    |
| Methyl salicylate                                    | 454                             |                                                                                 |       |
| $\alpha$ -Methylstyrene                              | 574                             | 1.9                                                                             | 6.1   |
| Methyl vinyl ether                                   |                                 | 2.6                                                                             | 39    |
| Morpholine                                           | 290                             | 1                                                                               | 11    |
| Naphtha, coal tar                                    | 277                             |                                                                                 |       |
| Naphthalene                                          | 526                             | 0.9                                                                             | 5.9   |
| Neoprene                                             |                                 | 4.0                                                                             | 20    |
| Nicotine                                             | 244                             | 0.75                                                                            | 4.0   |
| Nitrobenzene                                         | 482                             | 1.8                                                                             | 9     |
| 2-Nitrobiphenyl                                      | 179                             |                                                                                 |       |
| Nitroethane                                          | 414                             | 3.4                                                                             | 17    |
| Nitroglycerine                                       | 270                             |                                                                                 |       |
| Nitromethane                                         | 418                             | 7.3                                                                             | 22    |
| 1-Nitropropane                                       | 421                             | 2.2                                                                             |       |
| 2-Nitropropane                                       | 428                             | 2.6                                                                             | 11    |
| Nonane                                               | 205                             | 0.8                                                                             | 2.9   |
| Octadecanoic acid (stearic acid)                     | 395                             |                                                                                 |       |
| <i>cis</i> -9-Octadecenoic acid (oleic acid)         | 362                             |                                                                                 |       |
| Octane                                               | 206                             | 1.0                                                                             | 6.5   |
| 1-Octene                                             | 230                             |                                                                                 |       |
| Paraldehyde                                          | 238                             | 1.3                                                                             |       |
| Pentaborane(9)                                       |                                 | 0.42                                                                            |       |
| Pentanamine                                          |                                 | 2.2                                                                             | 22    |

**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                                 | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|-------------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                           |                                 | Lower                                                                           | Upper |
| Pentane                                   | 260                             | 1.5                                                                             | 7.8   |
| 1,5-Pentanediol                           | 335                             |                                                                                 |       |
| Pentanoic acid                            | 400                             |                                                                                 |       |
| 1-Pentanol                                | 300                             | 1.2                                                                             | 10.0  |
| 2-Pentanol                                | 343                             |                                                                                 |       |
| 3-Pentanol                                | 435                             | 1.2                                                                             | 9.0   |
| 2-Pentanone (methyl propyl ketone)        | 452                             | 1.5                                                                             | 8.2   |
| 3-Pentanone (diethyl ketone)              | 450                             | 1.6                                                                             |       |
| 1-Pentene                                 | 275                             | 1.5                                                                             | 8.7   |
| Pentyl acetate                            | 360                             | 1.1                                                                             | 7.5   |
| Pentylamine                               |                                 | 2.2                                                                             | 22    |
| Petroleum ether (solvent naphtha)         | 288                             | 1.1                                                                             | 5.9   |
| Phenol                                    | 715                             | 1.8                                                                             | 8.6   |
| Phosphorus, red                           | 260                             |                                                                                 |       |
| Phosphorus, white                         | 30                              |                                                                                 |       |
| Phosphorus pentasulfide                   | 142                             |                                                                                 |       |
| o-Phthalic anhydride                      | 570                             | 1.7                                                                             | 10.4  |
| Picric acid                               | 300 (explodes)                  |                                                                                 |       |
| α-Pinene                                  | 275                             |                                                                                 |       |
| β-Pinene                                  | 275                             |                                                                                 |       |
| Piperidine                                |                                 | 1                                                                               | 10    |
| 1-Propanal                                | 207                             | 2.6                                                                             | 17    |
| 1-Propanamine (propylamine)               | 318                             | 2.0                                                                             | 10.4  |
| Propane                                   | 450                             | 2.1                                                                             | 9.5   |
| 1,2-Propanediol                           | 371                             | 2.6                                                                             | 12.5  |
| 1,3-Propanediol                           | 400                             |                                                                                 |       |
| Propanenitrile                            | 512                             | 3.1                                                                             | 14    |
| 1,2,3-Propanetriol (glycerol)             | 370                             | 3                                                                               | 19    |
| 1,2,3-Propanetriol triacetate (triacetin) | 433                             | 1.0                                                                             |       |
| Propanoic acid                            | 465                             | 2.9                                                                             | 12.1  |
| Propanoic anhydride                       | 285                             | 1.3                                                                             | 9.5   |
| 1-Propanol                                | 412                             | 2.2                                                                             | 13.7  |
| 2-Propanol                                | 399                             | 2.0                                                                             | 12.7  |
| Propene                                   | 460                             | 2.4                                                                             | 10.1  |
| Propyl acetate                            | 450                             | 1.7                                                                             | 8     |
| Propylbenzene                             | 450                             | 0.8                                                                             | 6.0   |
| Propyl formate                            | 455                             |                                                                                 |       |
| Propyl nitrate                            | 175                             | 2                                                                               | 100   |
| Propyne                                   |                                 | 1.7                                                                             |       |
| Pyridine                                  | 482                             | 1.8                                                                             | 12.4  |
| Quinoline                                 | 480                             |                                                                                 |       |
| Sodium                                    | 115 (dry air)                   |                                                                                 |       |
| Styrene                                   | 490                             | 0.9                                                                             | 6.8   |
| Sulfur (di-) dichloride                   | 233                             |                                                                                 |       |
| 1,1,2,2-Tetrabromoethane                  | 335                             |                                                                                 |       |
| Tetrabromoethylene                        | 335                             |                                                                                 |       |
| 1,1,1,2-Tetrachloroethane                 |                                 | 5                                                                               | 12    |

**TABLE 5.23** Properties of Combustible Mixtures in Air (*Continued*)

| Substance                                         | Autoignition<br>temperature, °C | Flammable (explosive)<br>limits, percent by<br>volume of fuel (25°C,<br>760 mm) |       |
|---------------------------------------------------|---------------------------------|---------------------------------------------------------------------------------|-------|
|                                                   |                                 | Lower                                                                           | Upper |
| 1,1,2,2-Tetrachloroethane                         |                                 | 20                                                                              | 54    |
| Tetrahydrofuran                                   | 321                             | 2                                                                               | 11.8  |
| Tetrahydrofurfuryl alcohol                        | 282                             | 1.5                                                                             | 9.7   |
| 1,2,3,4-Tetrahydronaphthalene                     | 385                             | 0.8                                                                             | 5.0   |
| 2,2,3,3-Tetramethylpentane                        | 430                             | 0.8                                                                             | 4.9   |
| 2,2-Thiodiethanol                                 | 298                             |                                                                                 |       |
| Titanium, powder                                  | 250                             |                                                                                 |       |
| Toluene                                           | 480                             | 1.1                                                                             | 7.1   |
| Toluene diisocyanate                              |                                 | 0.9                                                                             | 9.5   |
| <i>o</i> -Toluidine (also <i>p</i> -)             | 482                             |                                                                                 |       |
| Tributylamine                                     |                                 | 1                                                                               | 5     |
| 1,1,1-Trichloroethane                             | 537                             | 7.5                                                                             | 12.5  |
| 1,1,2-Trichloroethane                             | 460                             | 6                                                                               | 28    |
| Trichloroethylene                                 | 420                             | 8                                                                               | 10.5  |
| (Trichloromethyl)benzene                          | 211                             |                                                                                 |       |
| Trichloromethylsilane                             | >404                            | 7.6                                                                             | >20   |
| 1,2,3-Trichloropropane                            |                                 | 3.2                                                                             | 12.6  |
| Trichlorosilane                                   | 104                             |                                                                                 |       |
| 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon 113) | 680                             |                                                                                 |       |
| Tri- <i>o</i> -cresyl phosphate                   | 385                             |                                                                                 |       |
| Triethanolamine                                   |                                 | 1                                                                               | 10    |
| Triethylamine                                     | 249                             | 1.2                                                                             | 8.0   |
| Triethylene glycol                                | 371                             | 0.9                                                                             | 9.2   |
| Triethyl phosphate                                | 454                             |                                                                                 |       |
| Trimethylamine                                    | 190                             | 2.0                                                                             | 11.6  |
| 1,2,3-Trimethylbenzene (hemimellitene)            | 470                             | 0.8                                                                             | 6.6   |
| 1,2,4-Trimethylbenzene (pseudocumene)             | 500                             | 0.9                                                                             | 6.4   |
| 1,3,5-Trimethylbenzene                            | 559                             | 1                                                                               | 5     |
| 2,2,3-Trimethylbutane                             | 412                             |                                                                                 |       |
| 1,1,3-Trimethyl-3-cyclohexen-5-one                | 462                             | 0.8                                                                             | 3.8   |
| 3,5,5-Trimethylcyclohex-2-ene-1-one               | 460                             | 0.8                                                                             | 3.8   |
| 2,2,3-Trimethylpentane                            | 346                             |                                                                                 |       |
| 2,2,4-Trimethylpentane                            | 418                             | 1.1                                                                             | 6.0   |
| 2,3,3-Trimethylpentane                            | 425                             |                                                                                 |       |
| Trioxane                                          | 414                             | 3.6                                                                             | 28.7  |
| Tri- <i>o</i> -tolyl phosphate                    | 385                             |                                                                                 |       |
| Turpentine                                        |                                 | 0.8                                                                             |       |
| Vinyl acetate                                     | 402                             | 2.6                                                                             | 13.4  |
| Vinyl bromide                                     | 530                             | 9                                                                               | 15    |
| Vinyl butanoate                                   |                                 | 1.4                                                                             | 8.8   |
| Vinyl chloride                                    | 472                             | 3.6                                                                             | 33.0  |
| 4-Vinyl-1-cyclohexene                             | 269                             |                                                                                 |       |
| Vinyl fluoride                                    |                                 | 2.6                                                                             | 21.7  |
| Vinylidene                                        | 573                             | 5.6                                                                             | 16.0  |
| <i>m</i> -Xylene                                  | 527                             | 1.1                                                                             | 7.0   |
| <i>o</i> -Xylene                                  | 463                             | 0.9                                                                             | 6.7   |
| <i>p</i> -Xylene                                  | 528                             | 1.1                                                                             | 7.0   |



5.8 THERMAL CONDUCTIVITY

TABLE 5.24 Thermal Conductivities of Gases as a Function of Temperature

The coefficient  $k$ , expressed in  $\text{J} \cdot \text{sec}^{-1} \cdot \text{cm}^{-1} \cdot \text{K}^{-1}$ , is the quantity of heat in joules, transmitted per second through a sample one centimeter in thickness and one square centimeter in area when the temperature difference between the two sides is one degree kelvin (or Celsius). The tabulated values are in microjoules. To convert to microcalories, divide values by 4.184. To convert to  $\text{mW} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ , divide values by 10.

| Substance             | Temperature, °C    |      |                    |     |     |     |     |                    |     |     |                    |
|-----------------------|--------------------|------|--------------------|-----|-----|-----|-----|--------------------|-----|-----|--------------------|
|                       | − 40               | − 20 | 0                  | 20  | 40  | 60  | 80  | 100                | 120 | 140 | 160                |
| Acetone               |                    | 80   | 95                 | 107 | 124 | 140 | 156 | 173                | 190 | 207 |                    |
| Acetaldehyde          |                    |      |                    | 109 | 126 | 142 | 159 | 176                | 195 |     |                    |
| Acetonitrile          |                    |      |                    |     |     | 112 | 124 | 137                | 151 | 166 |                    |
| Acetylene             | 118 <sup>−75</sup> |      | 184                | 205 | 224 | 248 | 269 | 290                |     |     |                    |
| Air                   |                    |      | 242                | 256 | 270 | 284 | 299 | 311                | 324 | 336 | 342 <sup>149</sup> |
| Ammonia               | 164 <sup>−60</sup> |      | 218                | 238 | 259 | 280 | 301 | 321                |     |     |                    |
| Argon                 |                    |      | 166                | 176 | 186 | 196 | 206 | 211                |     |     |                    |
| Benzene               |                    |      |                    |     |     | 126 | 146 | 165                | 184 | 205 | 226                |
| Boron trifluoride     |                    |      |                    | 186 |     |     |     |                    |     | 241 |                    |
| Bromine               |                    |      | 42                 | 45  | 50  | 54  | 59  |                    |     |     |                    |
| Bromomethane          |                    |      |                    |     | 82  | 94  | 104 | 117                |     |     |                    |
| 1-Butanamine          |                    |      | 135 <sup>6.5</sup> |     |     |     |     | 176 <sup>110</sup> |     |     |                    |
| Butane                |                    |      | 135                | 154 | 174 | 193 | 213 | 233                |     |     |                    |
| Carbon dioxide        |                    |      | 144                | 160 | 176 | 192 | 207 | 215                |     |     |                    |
| Carbon disulfide      |                    |      | 67                 | 76  | 85  |     |     |                    |     |     |                    |
| Carbon monoxide       |                    |      | 228                | 245 | 262 | 278 |     |                    |     |     |                    |
| Carbon tetrachloride  |                    |      | 59                 | 64  | 70  | 75  | 80  | 86                 |     |     | 109 <sup>184</sup> |
| Chlorine              | 64                 |      | 79                 | 85  | 93  | 100 |     |                    |     |     |                    |
| Chlorodifluorimethane |                    | 72   | 110                | 116 | 122 |     |     |                    |     |     |                    |
| Chloroethane          |                    | 103  | 90                 | 105 | 120 | 134 | 151 | 167                | 186 | 204 |                    |
| Chloroform            |                    |      |                    |     | 75  | 84  | 91  | 99                 | 107 | 116 |                    |
| Chloromethane         |                    |      | 84                 | 105 | 117 | 130 | 142 | 155                |     |     |                    |
| Cyclohexane           |                    |      | 77                 | 99  | 120 | 141 | 163 | 184                | 206 | 230 | 256                |
| Cyclopropane          |                    |      |                    |     |     | 192 | 218 | 243                | 270 |     |                    |

| Substance                     | Temperature, °C |      |      |      |                   |                   |      |                   |                   |     |                    |
|-------------------------------|-----------------|------|------|------|-------------------|-------------------|------|-------------------|-------------------|-----|--------------------|
|                               | − 40            | − 20 | 0    | 20   | 40                | 60                | 80   | 100               | 120               | 140 | 160                |
| Deuterium                     | 1150            | 1222 | 1297 | 1372 | 1448              | 1523              |      |                   |                   |     |                    |
| Deuterium oxide               |                 |      |      |      |                   |                   |      |                   | 263               |     | 358 <sup>220</sup> |
| Dibromomethane                |                 |      |      |      |                   |                   |      |                   | 74 <sup>110</sup> |     |                    |
| Dichlorodifluoromethane       |                 | 81   | 84   | 92   | 100               |                   |      | 138               |                   |     | 194 <sup>200</sup> |
| 1,1-Dichloroethane            |                 |      | 69   | 81   | 93                | 105               | 117  | 129               | 144               |     |                    |
| 1,2-Dichloroethane            |                 |      |      |      |                   |                   |      | 127               | 140               |     |                    |
| Dichlorofluoromethane         |                 | 91   | 94   | 97   | 100               |                   |      |                   |                   |     |                    |
| Dichloromethane               |                 |      | 93   |      |                   |                   |      | 161               |                   |     |                    |
| 1,2-Dichlorotetrafluoroethane |                 |      |      | 99   |                   |                   |      |                   | 153               |     | 211 <sup>227</sup> |
| Diethylamine                  |                 |      | 118  |      |                   | 179               | 199  | 218               | 243               | 268 |                    |
| Diethyl ether                 |                 |      | 113  | 135  | 157               | 178               | 200  | 222               | 244               | 269 | 351 <sup>213</sup> |
| 1,4-Dioxane                   |                 |      |      |      |                   |                   |      | 167               | 187               | 207 |                    |
| Ethane                        | 137             | 159  | 182  | 204  | 228               | 257               | 288  | 316               | 344               |     |                    |
| Ethanol                       |                 |      | 126  | 141  | 155               |                   |      | 209               |                   |     |                    |
| Ethene                        |                 |      |      |      | 230 <sup>49</sup> |                   |      |                   |                   |     |                    |
| Ethyl acetate                 |                 |      |      |      | 115               | 133               | 151  | 170               | 191               | 211 | 234                |
| Ethylamine                    |                 |      | 136  | 153  | 169               | 206               |      |                   |                   |     |                    |
| Ethylene                      | 137             | 158  | 178  | 220  | 241               | 262               | 282  |                   |                   |     |                    |
| Ethylene oxide                |                 |      |      |      |                   |                   |      | 193               | 256               | 279 |                    |
| Ethyl formate                 |                 |      | 79   | 100  | 121               | 142               | 164  | 186               | 206               | 226 |                    |
| Ethyl nitrate                 |                 |      |      |      |                   |                   |      | 159               | 178               | 197 |                    |
| Fluorine                      | 212             | 230  | 247  | 264  | 278               | 294               | 309  | 325               |                   |     |                    |
| Helium                        | 1276            | 1343 | 1423 | 1481 | 1540              | 1598              | 1661 | 1720              | 1778              |     |                    |
| Heptane                       |                 |      | 100  | 115  | 130               |                   |      | 174               |                   |     |                    |
| Hexane                        |                 |      | 109  |      |                   |                   | 178  | 201               | 224               | 247 | 271                |
| Hydrogen                      | 1494            | 1607 | 1724 | 1828 | 1925              | 2025              |      |                   |                   |     |                    |
| Hydrogen bromide              | 64              | 70   | 77   | 84   | 90                | 97                | 104  |                   |                   |     |                    |
| Hydrogen chloride             | 107             | 117  | 128  | 138  | 148               |                   |      |                   | 191               |     | 240 <sup>227</sup> |
| Hydrogen cyanide              |                 | 99   | 110  | 121  | 132               | 143               |      |                   |                   |     |                    |
| Hydrogen sulfide              |                 | 116  | 129  | 143  | 156               | 169               |      |                   |                   |     |                    |
| Iodomethane                   |                 |      | 46   | 53   | 60                | 68                | 75   | 82                | 89                |     |                    |
| Krypton                       |                 | 79   | 85   |      | 95                |                   |      | 110               |                   |     |                    |
| Methane                       | 257             | 280  | 307  | 334  | 361               | 387               | 416  | 445               |                   |     |                    |
| Methanol                      |                 |      |      |      |                   | 174               | 197  | 221               | 241               | 263 | 284                |
| Methyl acetate                |                 |      | 67   |      |                   | 150 <sup>70</sup> |      | 177               | 195               | 215 | 237                |
| 2-Methylbutane                |                 |      | 122  |      |                   |                   |      | 215               |                   |     |                    |
| 2-Methylpropane               |                 |      | 141  | 156  | 176               | 196               |      | 233 <sup>93</sup> | 271               |     | 421 <sup>227</sup> |

**TABLE 5.24** Thermal Conductivities of Gases as a Function of Temperature (*Continued*)

| Substance                      | Temperature, °C   |      |     |                   |     |     |     |                    |     |                    |                    |
|--------------------------------|-------------------|------|-----|-------------------|-----|-----|-----|--------------------|-----|--------------------|--------------------|
|                                | − 40              | − 20 | 0   | 20                | 40  | 60  | 80  | 100                | 120 | 140                | 160                |
| 2-Methyl-2-propanol            |                   |      |     |                   |     |     |     | 225                |     |                    |                    |
| Neon                           | 410               | 433  | 454 | 476               | 497 | 518 | 537 | 556                |     |                    |                    |
| Nitric oxide                   | 205               | 221  | 238 | 254               | 269 | 285 | 301 | 317                |     |                    |                    |
| Nitrogen                       | 211               | 226  | 241 | 256               | 270 | 282 | 295 | 307                | 320 | 333                | 385 <sup>227</sup> |
| Nitromethane                   |                   |      |     |                   |     |     |     |                    | 139 | 155                |                    |
| Nitrous oxide                  | 121               | 137  | 152 | 168               | 184 |     |     |                    |     |                    |                    |
| Octafluorocyclobutane          |                   |      |     | 120               |     |     |     |                    | 190 |                    |                    |
| Oxygen                         | 211               | 228  | 245 | 261               | 278 | 294 | 311 | 328                |     |                    |                    |
| Pentane                        |                   |      | 130 |                   |     |     |     | 218                |     |                    |                    |
| Propane                        | 116               | 132  | 151 | 171               | 192 | 215 | 238 | 262                | 330 | 353                | 379                |
| 2-Propanol                     |                   |      |     | 151 <sup>31</sup> |     |     |     |                    |     | 250 <sup>127</sup> |                    |
| Sulfur dioxide                 |                   |      | 83  |                   | 163 |     |     | 106                |     |                    |                    |
| Sulfur hexafluoride            |                   |      |     | 126               |     |     |     |                    | 201 | 275 <sup>227</sup> | 338 <sup>327</sup> |
| Tetrafluoromethane             |                   |      |     | 235               |     |     |     |                    | 235 |                    |                    |
| Thiophene                      |                   |      |     |                   |     |     |     | 152 <sup>110</sup> |     |                    |                    |
| 1,1,2-Trichlorotrifluoroethane |                   |      |     | 87                |     |     |     |                    | 133 |                    |                    |
| Triethylamine                  |                   |      |     |                   |     |     |     | 195                | 216 | 239                |                    |
| Water                          |                   | 142  | 159 | 175               | 191 | 207 | 224 | 241                | 257 |                    |                    |
| Xenon                          | 36 <sup>−73</sup> |      |     | 54                |     |     |     |                    | 72  | 89 <sup>227</sup>  | 104 <sup>327</sup> |

**TABLE 5.25** Liquid Thermal Conductivity of Various Substances

All values of thermal conductivity,  $k$ , are in millijoules  $\text{cm}^{-1} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$ . To convert to  $\text{mJ} \cdot \text{cm}^{-1} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$  into  $\text{mW} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ , divide by 10.

| Substance                     | Thermal conductivity in $\text{mJ} \cdot \text{cm}^{-1} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$ |                     |                    |                     |                    |                     |       |
|-------------------------------|--------------------------------------------------------------------------------------------------|---------------------|--------------------|---------------------|--------------------|---------------------|-------|
|                               | − 25°C                                                                                           | 0°C                 | 20°C               | 25°C                | 50°C               | 75°C                | 100°C |
| Acetaldehyde                  |                                                                                                  |                     | 1.900              |                     |                    |                     |       |
| Acetic acid                   |                                                                                                  |                     |                    | 1.58                | 1.53               | 1.49                | 1.44  |
| Acetic anhydride              |                                                                                                  |                     | 2.209              |                     |                    |                     |       |
| Acetone                       | 1.987 <sup>−80</sup>                                                                             | 1.69                | 1.61               |                     | 1.51 <sup>40</sup> |                     |       |
| Acetonitrile                  | 2.08                                                                                             | 1.98                |                    | 1.88                | 1.78               | 1.68                |       |
| Allyl alcohol                 |                                                                                                  |                     |                    | 1.80 <sup>30</sup>  |                    |                     |       |
| Aniline                       |                                                                                                  |                     | 1.77 <sup>17</sup> |                     |                    |                     |       |
| Argon                         | 1.259 <sup>−189</sup>                                                                            |                     |                    |                     |                    |                     |       |
| Benzaldehyde                  |                                                                                                  |                     |                    | 1.51                | 1.41               | 1.31                | 1.21  |
| Benzene                       |                                                                                                  |                     |                    | 1.411               | 1.329              | 1.247               |       |
| Bromobenzene                  |                                                                                                  |                     | 1.113              |                     |                    |                     |       |
| Bromoethane                   |                                                                                                  |                     | 1.029              |                     |                    |                     |       |
| 1-Bromo-2-methylpropane       |                                                                                                  | 1.163 <sup>12</sup> |                    |                     |                    |                     |       |
| 1-Bromopentane                |                                                                                                  |                     | 0.983              |                     |                    |                     |       |
| Bromopropane                  |                                                                                                  | 1.075 <sup>12</sup> |                    |                     |                    |                     |       |
| Butanoic acid                 |                                                                                                  | 1.506 <sup>12</sup> |                    |                     |                    |                     |       |
| 1-Butanol                     |                                                                                                  | 1.538               |                    | 1.54                | 1.49               |                     |       |
| 2-Butanone                    | 1.58                                                                                             | 1.51                |                    | 1.45                | 1.39               | 1.33                |       |
| Butyl acetate                 |                                                                                                  |                     | 1.368              |                     |                    |                     |       |
| 2-Butyne                      | 1.37                                                                                             | 1.29                |                    | 1.21                |                    |                     |       |
| Carbon disulfide              |                                                                                                  | 1.54                |                    | 1.49                |                    |                     |       |
| Carbon tetrachloride          | 1.100 <sup>−20</sup>                                                                             | 1.071               | 1.029              |                     | 0.974              |                     |       |
| Chlorobenzene                 | 1.36                                                                                             | 1.31                |                    | 1.27                | 1.22               | 1.17                | 1.12  |
| Chloroethane                  | 1.45                                                                                             | 1.32                |                    | 1.19                | 1.06               | 0.93                |       |
| Chloroform                    | 1.27                                                                                             | 1.22                |                    | 1.17                | 1.12               | 1.07                | 1.02  |
| (Chloromethyl)oxirane         | 1.42                                                                                             | 1.37                |                    | 1.31                | 1.25               | 1.19                | 1.14  |
| 1-Chloro-2-methylpropane      |                                                                                                  | 1.163 <sup>12</sup> |                    |                     |                    |                     |       |
| 1-Chloropentane               |                                                                                                  | 1.184 <sup>12</sup> |                    |                     |                    |                     |       |
| Chloropropane                 |                                                                                                  | 1.184 <sup>12</sup> |                    |                     |                    |                     |       |
| 4-Chlorotoluene               |                                                                                                  |                     | 1.297              |                     |                    |                     |       |
| <i>m</i> -Cresol              |                                                                                                  |                     | 1.498              |                     |                    | 1.452 <sup>80</sup> |       |
| Cyclohexane                   |                                                                                                  |                     | 1.243              | 1.23                | 1.17               | 1.11                |       |
| Cyclohexene                   | 1.42                                                                                             | 1.36                |                    | 1.30                | 1.24               | 1.18                |       |
| Cyclohexanol                  |                                                                                                  |                     |                    | 1.34                | 1.31               |                     |       |
| Cyclopentane                  | 1.40                                                                                             | 1.33                |                    | 1.26                |                    |                     |       |
| Cyclopentene                  | 1.43                                                                                             | 1.36                |                    | 1.29                |                    |                     |       |
| Decane                        | 1.44                                                                                             | 1.38                |                    | 1.32                | 1.26               | 1.19                | 1.13  |
| 1-Decanol                     |                                                                                                  |                     |                    | 1.62                | 1.56               | 1.50                | 1.45  |
| Dibromomethane                | 1.20                                                                                             | 1.14                |                    | 1.08                | 1.03               | 0.97                |       |
| Dibutyl phthalate             | 1.44                                                                                             | 1.40                |                    | 1.36                | 1.33               | 1.29                | 1.25  |
| 1,2-Dichloroethane            |                                                                                                  | 1.264               |                    |                     |                    |                     |       |
| Dichlorofluoromethane         | 0.134                                                                                            |                     |                    |                     |                    |                     |       |
| Dichloromethane               | 1.590 <sup>−20</sup>                                                                             | 1.564               | 1.477              |                     |                    |                     |       |
| Diethyl ether                 | 1.50                                                                                             | 1.40                |                    | 1.30                | 1.20               | 1.10                | 1.00  |
| Diisopropyl ether             |                                                                                                  |                     | 1.096              |                     |                    |                     |       |
| 2,3-Dimethylbutane            |                                                                                                  |                     |                    | 1.038 <sup>32</sup> | 0.996              |                     |       |
| <i>N,N</i> -Dimethylformamide |                                                                                                  |                     |                    | 1.84                | 1.78               | 1.71                | 1.65  |
| Dimethyl phthalate            |                                                                                                  | 1.501               |                    | 1.473               | 1.443              | 1.409               | 1.373 |

TABLE 5.25 Liquid Thermal Conductivity of Various Substances (Continued)

| Substance                   | Thermal conductivity in $\text{mJ} \cdot \text{cm}^{-1} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$ |                     |                      |                      |                      |                      |                       |
|-----------------------------|--------------------------------------------------------------------------------------------------|---------------------|----------------------|----------------------|----------------------|----------------------|-----------------------|
|                             | $-25^{\circ}\text{C}$                                                                            | $0^{\circ}\text{C}$ | $20^{\circ}\text{C}$ | $25^{\circ}\text{C}$ | $50^{\circ}\text{C}$ | $75^{\circ}\text{C}$ | $100^{\circ}\text{C}$ |
| 1,4-Dioxane                 |                                                                                                  |                     |                      | 1.59                 | 1.47                 | 1.35                 | 1.23                  |
| Diphenyl ether              |                                                                                                  |                     |                      |                      | 1.39                 | 1.35                 | 1.31                  |
| Dodecane                    |                                                                                                  | 1.57                |                      | 1.52                 | 1.46                 | 1.40                 | 1.35                  |
| 1-Dodecanol                 |                                                                                                  |                     |                      | 1.46                 | 1.42                 | 1.39                 | 1.35                  |
| Ethanol                     |                                                                                                  | 1.76                |                      | 1.69                 | 1.62                 |                      |                       |
| Ethanolamine                |                                                                                                  |                     |                      | 2.99                 | 2.86                 | 2.74                 | 2.61                  |
| Ethoxybenzene               |                                                                                                  |                     | 1.497                |                      |                      |                      |                       |
| Ethyl acetate               | 1.62                                                                                             | 1.53                |                      | 1.44                 | 1.35                 | 1.26                 |                       |
| Ethylbenzene                |                                                                                                  |                     |                      | 1.30                 | 1.24                 | 1.18                 | 1.12                  |
| Ethylene glycol             |                                                                                                  | 2.56                |                      | 2.56                 | 2.56                 | 2.56                 | 2.56                  |
| Ethyl formate               |                                                                                                  | 1.581 <sup>12</sup> |                      |                      |                      |                      |                       |
| Furan                       | 1.42                                                                                             | 1.34                |                      | 1.26                 |                      |                      |                       |
| Glycerol                    |                                                                                                  |                     |                      | 2.92                 | 2.95                 | 2.97                 | 3.00                  |
| Heptane                     | 1.378                                                                                            | 1.303               | 1.259                | 1.228                | 1.152                | 1.077                |                       |
| 1-Heptanol                  |                                                                                                  | 1.66                |                      | 1.59                 | 1.53                 | 1.47                 | 1.41                  |
| Hexadecane                  |                                                                                                  |                     |                      | 1.40                 | 1.35                 | 1.30                 | 1.25                  |
| Hexane                      | 1.37                                                                                             | 1.28                | 1.218                | 1.20                 | 1.11                 | 1.92                 | 0.93                  |
| 1-Hexanol                   | 1.59                                                                                             | 1.54                |                      | 1.50                 | 1.45                 | 1.41                 | 1.37                  |
| 2-Hexanone                  | 1.51                                                                                             | 1.45                |                      | 1.39                 | 1.33                 | 1.27                 | 1.21                  |
| 1-Hexene                    | 1.37                                                                                             | 1.29                |                      | 1.21                 | 1.13                 |                      |                       |
| Hydrochloric acid, 38%      |                                                                                                  |                     | 4.402 <sup>32</sup>  |                      |                      |                      |                       |
| Hydrogen                    | 1.180 <sup>-253</sup>                                                                            |                     |                      |                      |                      |                      |                       |
| Iodobenzene                 | 1.063 <sup>-20</sup>                                                                             |                     | 1.276                |                      |                      | 0.937 <sup>80</sup>  |                       |
| Iodoethane                  |                                                                                                  |                     |                      | 1.109 <sup>30</sup>  |                      |                      |                       |
| 1-Iodo-2-methylpropane      |                                                                                                  | 0.870 <sup>12</sup> |                      |                      |                      |                      |                       |
| 1-Iodopentane               |                                                                                                  | 0.849 <sup>12</sup> |                      |                      |                      |                      |                       |
| Iodopropane                 |                                                                                                  | 0.920 <sup>12</sup> |                      |                      |                      |                      |                       |
| Isopentyl acetate           |                                                                                                  |                     | 1.297                |                      |                      |                      |                       |
| Isopropylbenzene            |                                                                                                  |                     |                      | 1.28                 | 1.20                 | 1.12                 | 1.07                  |
| Mercury                     | 72.5                                                                                             | 77.7                |                      | 82.5                 | 86.8                 | 90.7                 | 94.3                  |
| Methanol                    | 2.14                                                                                             | 2.07                | 2.021                | 2.00                 | 1.93                 |                      |                       |
| Methoxybenzene              | 1.70                                                                                             | 1.63                |                      | 1.56                 | 1.50                 | 1.43                 | 1.36                  |
| Methyl acetate              | 1.74                                                                                             | 1.64                |                      | 1.53                 | 1.43                 | 1.33                 | 1.22                  |
| Methyl butanoate            |                                                                                                  |                     | 1.402                |                      |                      |                      |                       |
| 3-Methylbutanoic acid       |                                                                                                  | 1.305               |                      |                      |                      |                      |                       |
| 3-Methyl-1-butanol          |                                                                                                  |                     |                      | 1.477 <sup>30</sup>  |                      |                      |                       |
| Methylcyclohexane           |                                                                                                  |                     |                      | 1.276 <sup>30</sup>  |                      |                      |                       |
| Methylcyclopentane          |                                                                                                  |                     |                      | 1.209                | 1.151 <sup>38</sup>  |                      |                       |
| N-Methylformamide           |                                                                                                  |                     |                      | 2.03                 | 2.01                 | 1.99                 | 1.96                  |
| 1-Methyl-4-isopropylbenzene | 1.32                                                                                             | 1.27                |                      | 1.22                 | 1.17                 | 1.12                 | 1.07                  |
| 2-Methylpentane             |                                                                                                  |                     |                      | 1.084 <sup>32</sup>  | 1.033                |                      |                       |
| Methyl pentanoate           |                                                                                                  | 1.318 <sup>12</sup> |                      |                      |                      |                      |                       |
| 4-Methylpentanoic acid      |                                                                                                  | 1.427 <sup>12</sup> |                      |                      |                      |                      |                       |
| 4-Methyl-3-pentene-2-one    | 1.70                                                                                             | 1.63                |                      | 1.56                 | 1.49                 | 1.42                 | 1.34                  |
| 2-Methyl-1-propanol         |                                                                                                  | 1.423 <sup>12</sup> |                      |                      |                      |                      |                       |
| 2-Methyl-2-propanol         |                                                                                                  |                     |                      | 1.159 <sup>38</sup>  |                      | 1.067 <sup>77</sup>  |                       |
| Nitrobenzene                |                                                                                                  |                     | 1.510                |                      |                      |                      |                       |
| Nitromethane                |                                                                                                  |                     |                      | 2.151 <sup>30</sup>  |                      |                      |                       |
| Nonane                      | 1.44                                                                                             | 1.38                |                      | 1.31                 | 1.24                 | 1.151 <sup>80</sup>  | 1.11                  |

**TABLE 5.25** Liquid Thermal Conductivity of Various Substances (*Continued*)

| Substance                  | Thermal conductivity in $\text{mJ} \cdot \text{cm}^{-1} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$ |                     |       |                     |                     |                     |                      |
|----------------------------|--------------------------------------------------------------------------------------------------|---------------------|-------|---------------------|---------------------|---------------------|----------------------|
|                            | − 25°C                                                                                           | 0°C                 | 20°C  | 25°C                | 50°C                | 75°C                | 100°C                |
| 1-Nonanol                  |                                                                                                  | 1.66                |       | 1.61                | 1.55                | 1.49                | 1.43                 |
| Octadecane                 |                                                                                                  |                     |       |                     | 1.46                | 1.42                | 1.37                 |
| Octane                     | 1.43                                                                                             | 1.35                |       | 1.28                | 1.20                | 1.13                | 1.06                 |
| 1-Octanol                  |                                                                                                  | 1.68                | 1.657 | 1.61                | 1.54                | 1.47                | 1.41                 |
| Palmitic acid              |                                                                                                  |                     |       |                     |                     | 1.598               |                      |
| Pentachloroethane          |                                                                                                  |                     | 1.251 |                     |                     |                     |                      |
| Pentane                    | 1.32                                                                                             | 1.22                | 1.138 | 1.13                | 1.03                | 0.95                | 0.87                 |
| Pentanoic acid             |                                                                                                  | 1.360 <sup>12</sup> |       |                     |                     |                     |                      |
| 1-Pentanol                 |                                                                                                  | 1.57                |       | 1.53                | 1.49                | 1.45                |                      |
| 1-Pentene                  | 1.31                                                                                             | 1.24                |       | 1.16                |                     |                     |                      |
| Pentyl acetate             |                                                                                                  |                     | 1.289 |                     |                     |                     |                      |
| Phenol                     |                                                                                                  |                     |       |                     | 1.56                | 1.53                | 1.51                 |
| Phenylhydrazine            |                                                                                                  |                     |       | 1.724               |                     |                     |                      |
| 1,2-Propanediol            |                                                                                                  | 2.02                |       | 2.00                | 1.99                | 1.98                | 1.97                 |
| Propanoic acid             |                                                                                                  | 1.728 <sup>12</sup> |       |                     |                     |                     |                      |
| 1-Propanol                 | 1.62                                                                                             | 1.58                |       | 1.54                | 1.49                | 1.45                | 1.41                 |
| 2-Propanol                 | 1.46                                                                                             | 1.41                |       | 1.35                | 1.29                | 1.24                | 1.18                 |
| 1,2-Propylene glycol       |                                                                                                  | 2.008               |       |                     |                     |                     |                      |
| Propyl formate             |                                                                                                  | 1.494 <sup>12</sup> |       |                     |                     |                     |                      |
| Pyridine                   |                                                                                                  | 1.69                |       | 1.65                | 1.61                | 1.58                |                      |
| Silicon tetrachloride      |                                                                                                  |                     |       | 0.99                | 0.96                |                     |                      |
| Sodium                     |                                                                                                  |                     |       |                     |                     |                     | 753.1 <sup>300</sup> |
| Sodium chloride (aq, satd) | 5.732                                                                                            |                     |       |                     |                     |                     |                      |
| Stearic acid               |                                                                                                  |                     |       |                     |                     | 1.598               |                      |
| Styrene                    | 1.48                                                                                             | 1.42                |       | 1.37                | 1.31                | 1.26                | 1.20                 |
| Sulfuric acid, 90%         |                                                                                                  |                     |       | 3.540 <sup>32</sup> |                     |                     |                      |
| 1,1,2,2-Tetrachloroethane  |                                                                                                  | 1.138               |       |                     |                     |                     |                      |
| Tetrachloroethylene        | 1.17                                                                                             |                     | 1.10  | 1.04                | 0.97                |                     |                      |
| Tetrachloromethane         | 1.04                                                                                             |                     | 0.99  | 0.93                | 0.88                |                     |                      |
| Tetradecane                |                                                                                                  |                     |       | 1.36                | 1.31                | 1.26                | 1.21                 |
| 1-Tetradecanol             |                                                                                                  |                     |       |                     | 1.67                | 1.62                | 1.57                 |
| Tetrahydrofuran            | 1.32                                                                                             | 1.26                |       | 1.20                | 1.14                |                     |                      |
| Thiophene                  |                                                                                                  |                     |       | 1.99                | 1.95                | 1.91                | 1.86                 |
| Toluene                    | 1.590 <sup>-80</sup>                                                                             | 1.386               | 1.347 | 1.311               | 1.236               | 1.161               |                      |
| 1,1,1-Trichloroethane      | 1.06                                                                                             |                     | 1.01  | 0.96                |                     |                     |                      |
| Trichloroethylene          | 1.359 <sup>-60</sup>                                                                             | 1.24                |       | 1.160               | 1.08                | 1.00                |                      |
| Trichloromethane           | 1.27                                                                                             | 1.22                |       | 1.17                | 1.12                | 1.07                |                      |
| Tridecane                  |                                                                                                  |                     |       | 1.37                | 1.32                | 1.27                | 1.22                 |
| Triethylamine              | 1.464 <sup>-80</sup>                                                                             |                     | 1.209 |                     | 1.113 <sup>44</sup> |                     |                      |
| Trimethylamine             | 1.43                                                                                             | 1.33                |       |                     |                     |                     |                      |
| 1,3,5-Trimethylbenzene     | 1.47                                                                                             | 1.41                |       | 1.36                | 1.30                | 1.24                | 1.18                 |
| 2,2,4-Trimethylpentane     |                                                                                                  |                     |       | 0.966 <sup>38</sup> |                     | 0.841 <sup>77</sup> |                      |
| Undecane                   |                                                                                                  |                     |       | 1.40                | 1.35                | 1.29                | 1.23                 |
| Water                      |                                                                                                  | 5.610               | 5.983 | 6.071               | 6.435               | 6.668               | 6.791                |
| <i>m</i> -Xylene           |                                                                                                  |                     |       | 1.30                | 1.24                | 1.18                | 1.13                 |
| <i>o</i> -Xylene           |                                                                                                  |                     |       | 1.31                | 1.26                | 1.20                | 1.14                 |
| <i>p</i> -Xylene           |                                                                                                  |                     |       | 1.30                | 1.24                | 1.18                | 1.12                 |

TABLE 5.26 Thermal Conductivity of Various Solids

All values of thermal conductivity,  $k$ , are in millijoules  $\text{cm}^{-1} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$ . To convert to  $\text{mW} \cdot \text{m}^{-1} \cdot \text{K}^{-1}\text{m}$ , divide values by 10. For values in millicalories, divide by 4.184.

| Substance                               | $t, ^\circ\text{C}$ | $k$   |
|-----------------------------------------|---------------------|-------|
| Asphalt                                 | 20                  | 7.447 |
| Basalt                                  | 20                  | 21.76 |
| Bauxite                                 | 600                 | 5.56  |
| Boiler scale                            | 66                  | 13.1  |
| Brick, common                           | 20                  | 6.3   |
| Blotting paper                          | 20                  | 0.628 |
| Cardboard                               | 20                  | 2.1   |
| Cement, Portland                        | 90                  | 2.97  |
| Chalk                                   | 20                  | 9.2   |
| Chemical elements, <i>see</i> Table 4.1 |                     |       |
| Coal                                    | 0                   | 1.69  |
| Concrete                                | 20                  | 9.2   |
| Cork, sp. grav. = 0.2                   | 30                  | 0.54  |
| Cork meal                               | 100                 | 0.556 |
| Cotton, sp. grav. = 0.081               | 0                   | 0.569 |
| Diatomaceous earth                      | 20                  | 0.54  |
| Ebonite                                 | 0                   | 1.58  |
| Eiderdown                               | 20                  | 0.046 |
| Feathers (with air)                     | 9                   | 0.238 |
| Feldspar                                | 20                  | 23.4  |
| Felt (dark gray)                        | 40                  | 0.623 |
| Fire brick                              | 20                  | 4.6   |
| Flannel                                 | 60                  | 0.148 |
| Flint                                   | 20                  | 10.0  |
| Glass, crown                            | 12.5                | 6.82  |
| flint                                   | 12.5                | 5.98  |
| Jena                                    | 22                  | 9.50  |
| quartz                                  | 0                   | 13.89 |
|                                         | 100                 | 19.12 |
| soda                                    | 20                  | 7.1   |
|                                         | 100                 | 7.5   |
| Granite                                 | 20                  | 34.2  |
| Graphite, sp. grav. = 1.58              | 50                  | 441.4 |
| Graphite powder, sp. grav. = 0.7        | 40                  | 11.92 |
| Gypsum                                  | 0                   | 13.0  |
| Horse hair, sp. grav. = 0.172           | 20                  | 0.510 |
| Ice                                     |                     | 23.8  |
| Leather, cowhide                        | 84                  | 1.76  |
| Linen                                   | 20                  | 0.879 |
| Magnesia brick                          | 20                  | 11.3  |
|                                         | 1130                | 30.1  |
| Marble, white                           |                     | 32.6  |
| Mica                                    | 41                  | 3.60  |
| Naphthalene                             | 0                   | 3.77  |
| Paper                                   | 20                  | 1.3   |
| Paraffin                                | 0                   | 2.88  |
| Plaster of Paris                        | 20                  | 2.93  |
| Porcelain                               | 95                  | 10.38 |
| Quartz, parallel to axis                | 0                   | 136.0 |
|                                         | 100                 | 90.0  |

**TABLE 5.26** Thermal Conductivity of Various Solids (*Continued*)

| Substance                                            | $t, ^\circ\text{C}$ | $k$   |
|------------------------------------------------------|---------------------|-------|
| Quartz, perpendicular to axis                        | 0                   | 72.43 |
|                                                      | 100                 | 55.77 |
| Plastics, <i>see</i> Section 10                      |                     |       |
| Roofing paper                                        | 0                   | 1.90  |
| Rubber, natural and synthetic, <i>see</i> Section 10 |                     |       |
| Sand, dry                                            | 20                  | 3.89  |
| Sandstone, sp. grav. = 2.259                         | 40                  | 18.37 |
| Silk, sp. grav. = 0.101                              | 0                   | 0.510 |
| Slate                                                | 20                  | 19.66 |
| Soil, dry                                            | 20                  | 1.38  |
| Wax, bees                                            | 20                  | 0.866 |
| Wood, maple, parallel to face                        | 20                  | 4.25  |
| perpendicular to face                                | 50                  | 1.82  |
| Wood, oak, parallel to face                          | 15                  | 3.49  |
| perpendicular to face                                | 15                  | 2.09  |
| Wood, pine, parallel to face                         | 20                  | 3.49  |
| perpendicular to face                                | 15                  | 1.51  |

## 5.9 MISCELLANY

**TABLE 5.27** Compressibility of Water

In the table below are given the relative volumes of water at various temperatures and pressures. The volume at  $0^\circ\text{C}$  and one normal atmosphere (760 mm of Hg) is taken as unity.

| P, atm | $-10^\circ\text{C.}$ | $0^\circ\text{C.}$ | $10^\circ\text{C.}$ | $20^\circ\text{C.}$ | $40^\circ\text{C.}$ | $60^\circ\text{C.}$ | $80^\circ\text{C.}$ |
|--------|----------------------|--------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 1      | 1.0017               | 1.0000             | 1.0001              | 1.0016              | 1.0076              | 1.0168              | 1.0287              |
| 500    | 0.9788               | 0.9767             | 0.9778              | 0.9804              | 0.9867              | 0.9967              | 1.0071              |
| 1000   | 0.9581               | 0.9566             | 0.9591              | 0.9619              | 0.9689              | 0.9780              | 0.9884              |
| 1500   | 0.9399               | 0.9394             | 0.9424              | 0.9456              | 0.9529              | 0.9617              | 0.9717              |
| 2000   | 0.9223               | 0.9241             | 0.9277              | 0.9312              | 0.9386              | 0.9472              | 0.9568              |
| 2500   | 0.9083               | 0.9112             | 0.9147              | 0.9183              | 0.9257              | 0.9343              | 0.9437              |
| 3000   | 0.8962               | 0.8993             | 0.9028              | 0.9065              | 0.9139              | 0.9225              | 0.9315              |
| 3500   | 0.8852               | 0.8884             | 0.8919              | 0.8956              | 0.9030              | 0.9115              | 0.9203              |
| 4000   | 0.8751               | 0.8783             | 0.8818              | 0.8855              | 0.8931              | 0.9012              | 0.9097              |
| 4500   | 0.8658               | 0.8692             | 0.8725              | 0.8762              | 0.8838              | 0.8919              | 0.9001              |
| 5000   | 0.8573               | 0.8606             | 0.8639              | 0.8675              | 0.8752              | 0.8832              | 0.8913              |
| 6000   | .....                | 0.8452             | 0.8481              | 0.8517              | 0.8595              | 0.8674              | 0.8752              |
| 7000   | .....                | .....              | 0.8340              | 0.8374              | 0.8456              | 0.8534              | 0.8610              |
| 8000   | .....                | .....              | .....               | 0.8244              | 0.8330              | 0.8408              | 0.8483              |
| 9000   | .....                | .....              | .....               | 0.8128              | 0.8219              | 0.8297              | 0.8371              |
| 10000  | .....                | .....              | .....               | 0.8027              | 0.8119              | 0.8196              | 0.8268              |
| 11000  | .....                | .....              | .....               | .....               | 0.8023              | 0.8101              | 0.8172              |
| 12000  | .....                | .....              | .....               | .....               | 0.7931              | 0.8009              | 0.8080              |



**TABLE 5.28** Mass of Water Vapor in Saturated Air

The values in the table are grams of water contained in a cubic meter (m<sup>3</sup>) of saturated air at a total pressure 101 325 Pa (1 atm).

| °C  | g · m <sup>-3</sup> | °C | g · m <sup>-3</sup> | °C | g · m <sup>-3</sup> |
|-----|---------------------|----|---------------------|----|---------------------|
| -30 | 0.341               | 12 | 10.65               | 53 | 95.56               |
| -29 | 0.375               | 13 | 11.35               | 54 | 100.0               |
| -28 | 0.413               | 14 | 12.05               | 55 | 104.5               |
| -27 | 0.456               | 15 | 12.80               | 56 | 109.1               |
| -26 | 0.504               | 16 | 13.60               | 57 | 114.1               |
| -25 | 0.554               | 17 | 14.45               | 58 | 119.2               |
| -24 | 0.607               | 18 | 15.35               | 59 | 124.7               |
| -23 | 0.667               | 19 | 16.30               | 60 | 130.2               |
| -22 | 0.733               | 20 | 17.30               | 61 | 136.0               |
| -21 | 0.804               | 21 | 18.35               | 62 | 142.1               |
| -20 | 0.883               | 22 | 19.40               | 63 | 148.4               |
| -19 | 0.968               | 23 | 20.55               | 64 | 154.9               |
| -18 | 1.063               | 24 | 21.75               | 65 | 161.3               |
| -17 | 1.164               | 25 | 23.05               | 66 | 167.9               |
| -16 | 1.273               | 26 | 24.35               | 67 | 175.1               |
| -15 | 1.375               | 27 | 25.75               | 68 | 182.6               |
| -14 | 1.510               | 28 | 27.20               | 69 | 190.3               |
| -13 | 1.650               | 29 | 28.75               | 70 | 198.2               |
| -12 | 1.800               | 30 | 30.35               | 71 | 206.5               |
| -11 | 1.965               | 31 | 32.05               | 72 | 215.1               |
| -10 | 2.140               | 32 | 33.80               | 73 | 223.7               |
| -9  | 2.331               | 33 | 35.60               | 74 | 233.0               |
| -8  | 2.539               | 34 | 37.55               | 75 | 242.0               |
| -7  | 2.761               | 35 | 39.55               | 76 | 251.2               |
| -6  | 3.003               | 36 | 41.65               | 77 | 261.1               |
| -5  | 3.250               | 37 | 43.90               | 78 | 271.6               |
| -4  | 3.512               | 38 | 46.20               | 79 | 282.3               |
| -3  | 3.810               | 39 | 48.60               | 80 | 293.4               |
| -2  | 4.131               | 40 | 51.21               | 81 | 304.8               |
| -1  | 4.473               | 41 | 53.86               | 82 | 316.6               |
| 0   | 4.849               | 42 | 56.61               | 83 | 328.7               |
| 1   | 5.199               | 43 | 59.51               | 84 | 341.2               |
| 2   | 5.569               | 44 | 62.53               | 85 | 353.6               |
| 3   | 5.947               | 45 | 65.52               | 86 | 366.2               |
| 4   | 6.35                | 46 | 68.61               | 87 | 379.9               |
| 5   | 6.80                | 47 | 72.00               | 88 | 394.1               |
| 6   | 7.25                | 48 | 75.56               | 89 | 408.6               |
| 7   | 7.75                | 49 | 79.24               | 90 | 423.5               |
| 8   | 8.25                | 50 | 83.05               | 91 | 439.0               |
| 9   | 8.80                | 51 | 87.04               | 92 | 454.8               |
| 10  | 9.40                | 52 | 91.22               | 93 | 471.2               |
| 11  | 10.00               |    |                     |    |                     |

**TABLE 5.29** Van der Waals' Constants for Gases

The van der Waals' equation of state for a real gas is:

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT \quad \text{for } n \text{ moles}$$

where  $P$  is the pressure,  $V$  the volume (in liters per mole = 0.001 m<sup>3</sup> per mole in the SI system),  $T$  the temperature (in degrees Kelvin),  $n$  the amount of substance (in moles), and  $R$  the gas constant. To use the values of  $a$  and  $b$  in the table,  $P$  must be expressed in the same units as in the gas constant. Thus, the pressure of a standard atmosphere may be expressed in the SI system as follows:

$$1 \text{ atm} = 101,325 \text{ N} \cdot \text{m}^{-2} = 101,325 \text{ Pa} = 1.01325 \text{ bar}$$

The appropriate value for the gas constant is:

$$0.083\,144\,1 \text{ L} \cdot \text{bar} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \quad \text{or} \quad 0.082\,056 \text{ L} \cdot \text{atm} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

The van der Waals' constants are related to the critical temperature and pressure,  $t_c$  and  $P_c$ , in Table 6.5 by:

$$a = \frac{27 R^2 T_c^2}{64 P_c} \quad \text{and} \quad b = \frac{RT_c}{8 P_c}$$

| Substance                  | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|----------------------------|--------------------------------------------------------|-------------------------------------|
| Acetaldehyde               | 11.37                                                  | 0.08695                             |
| Acetic acid                | 17.71                                                  | 0.1065                              |
| Acetic anhydride           | 26.8                                                   | 0.157                               |
| Acetone                    | 16.02                                                  | 0.1124                              |
| Acetonitrile               | 17.89                                                  | 0.1169                              |
| Acetyl chloride            | 12.80                                                  | 0.08979                             |
| Acetylene                  | 4.516                                                  | 0.05218                             |
| Acrylic acid               | 19.45                                                  | 0.1127                              |
| Acrylonitrile              | 18.37                                                  | 0.1222                              |
| Allene                     | 8.235                                                  | 0.07467                             |
| Allyl alcohol              | 15.17                                                  | 0.1036                              |
| Aluminum trichloride       | 42.63                                                  | 0.2450                              |
| 2-Aminoethanol             | 7.616                                                  | 0.0431                              |
| Ammonia                    | 4.225                                                  | 0.03713                             |
| Ammonium chloride          | 2.380                                                  | 0.00734                             |
| Aniline                    | 29.14                                                  | 0.1486                              |
| Antimony tribromide        | 42.08                                                  | 0.1658                              |
| Argon                      | 1.355                                                  | 0.03201                             |
| Arsenic trichloride        | 17.23                                                  | 0.1039                              |
| Arsine                     | 6.327                                                  | 0.06048                             |
| Benzaldehyde               | 30.30                                                  | 0.1553                              |
| Benzene                    | 18.82                                                  | 0.1193                              |
| Benzonitrile               | 33.89                                                  | 0.1727                              |
| Benzyl alcohol             | 34.7                                                   | 0.173                               |
| Biphenyl                   | 47.16                                                  | 0.2130                              |
| Bismuth trichloride        | 33.89                                                  | 0.1025                              |
| Boron trichloride          | 15.60                                                  | 0.1222                              |
| Boron trifluoride          | 3.98                                                   | 0.05443                             |
| Bromine (Br <sub>2</sub> ) | 9.75                                                   | 0.0591                              |
| Bromobenzene               | 28.96                                                  | 0.1541                              |
| Bromochlorodifluoromethane | 12.79                                                  | 0.1055                              |
| Bromoethane                | 11.89                                                  | 0.08406                             |
| Bromomethane               | 6.753                                                  | 0.05390                             |
| Bromotrifluoromethane      | 8.502                                                  | 0.0891                              |

TABLE 5.29 Van der Waals' Constants for Gases (Continued)

| Substance                            | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|--------------------------------------|--------------------------------------------------------|-------------------------------------|
| 1,2-Butadiene                        | 12.76                                                  | 0.1025                              |
| 1,3-Butadiene                        | 12.17                                                  | 0.1020                              |
| Butanal                              | 19.48                                                  | 0.1292                              |
| Butane                               | 13.93                                                  | 0.1168                              |
| Butanenitrile                        | 25.76                                                  | 0.1568                              |
| Butanoic acid                        | 28.18                                                  | 0.1609                              |
| 1-Butanol                            | 20.90                                                  | 0.1323                              |
| 2-Butanol                            | 20.94                                                  | 0.1326                              |
| 2-Butanone                           | 19.97                                                  | 0.1326                              |
| 1-Butene                             | 12.76                                                  | 0.1084                              |
| cis-2-Butene                         | 12.58                                                  | 0.1066                              |
| trans-2-Butene                       | 12.58                                                  | 0.1066                              |
| 3-Butenenitrile                      | 25.76                                                  | 0.1568                              |
| Butyl acetate                        | 31.22                                                  | 0.1919                              |
| 1-Butylamine                         | 19.41                                                  | 0.1301                              |
| sec-Butylamine                       | 18.37                                                  | 0.1273                              |
| tert-Butylamine                      | 17.78                                                  | 0.1310                              |
| Butylbenzene                         | 44.071                                                 | 0.2378                              |
| sec-Butylbenzene                     | 43.74                                                  | 0.2347                              |
| tert-Butylbenzene                    | 42.77                                                  | 0.2310                              |
| Butyl benzoate                       | 57.97                                                  | 0.2857                              |
| Butylcyclohexane                     | 41.19                                                  | 0.2201                              |
| sec-Butylcyclohexane                 | 48.89                                                  | 0.2604                              |
| tert-Butylcyclohexane                | 48.34                                                  | 0.2614                              |
| Butyl ethyl ether                    | 27.05                                                  | 0.1815                              |
| 2-Butylhexadecafluorotetrahydrofuran | 45.41                                                  | 0.3235                              |
| 1-Butyne                             | 13.31                                                  | 0.1023                              |
| 2-Butyne                             | 13.68                                                  | 0.0998                              |
| Carbon dioxide                       | 3.658                                                  | 0.04284                             |
| Carbon disulfide                     | 11.25                                                  | 0.07262                             |
| Carbon monoxide                      | 1.472                                                  | 0.03948                             |
| Carbon oxysulfide (COS)              | 6.975                                                  | 0.06628                             |
| Carbon tetrachloride                 | 20.01                                                  | 0.1281                              |
| Carbon tetrafluoride                 | 4.029                                                  | 0.06319                             |
| Carbonyl chloride                    | 10.65                                                  | 0.08340                             |
| Carbonyl sulfide                     | 3.933                                                  | 0.05817                             |
| Chlorine                             | 6.343                                                  | 0.05422                             |
| Chlorine pentafluoride               | 9.581                                                  | 0.08214                             |
| Chlorobenzene                        | 25.80                                                  | 0.1454                              |
| 1-Chlorobutane                       | 23.22                                                  | 0.1527                              |
| 2-Chlorobutane                       | 20.01                                                  | 0.1370                              |
| 1-Chloro-1,1-difluoroethane          | 11.91                                                  | 0.1035                              |
| 2-Chloro-1,1-difluoroethylene        | 10.49                                                  | 0.09335                             |
| Chloroethane                         | 11.7                                                   | 0.090                               |
| Chloroform                           | 15.34                                                  | 0.1019                              |
| Chloromethane                        | 7.566                                                  | 0.06477                             |
| 2-Chloro-2-methylpropane             | 18.98                                                  | 0.1334                              |
| Chloropentafluoroacetone             | 17.08                                                  | 0.1482                              |
| Chloropentafluorobenzene             | 29.53                                                  | 0.1843                              |
| Chloropentafluoroethane              | 11.27                                                  | 0.1137                              |
| 1-Chloropropane                      | 16.11                                                  | 0.1141                              |
| 2-Chloropropane                      | 14.53                                                  | 0.1068                              |
| Chlorotrifluoromethane               | 6.873                                                  | 0.08110                             |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                                 | $a$ , L <sup>2</sup> · bar · mol <sup>-2</sup> | $b$ , L · mol <sup>-1</sup> |
|-------------------------------------------|------------------------------------------------|-----------------------------|
| Chlorotrifluorosilane                     | 7.994                                          | 0.09240                     |
| Chlorotrimethylsilane                     | 22.58                                          | 0.1617                      |
| <i>m</i> -Cresol                          | 31.86                                          | 0.1609                      |
| <i>o</i> -Cresol                          | 28.33                                          | 0.1447                      |
| <i>p</i> -Cresol                          | 28.11                                          | 0.1422                      |
| Cyanogen                                  | 7.803                                          | 0.06952                     |
| Cyclobutane                               | 12.39                                          | 0.0960                      |
| Cycloheptane                              | 27.20                                          | 0.1645                      |
| Cyclohexane                               | 21.95                                          | 0.1413                      |
| Cyclohexanol                              | 28.93                                          | 0.1586                      |
| Cyclohexanone                             | 31.1                                           | 0.170                       |
| Cyclohexene                               | 75.04                                          | 0.1339                      |
| Cyclopentane                              | 16.94                                          | 0.1180                      |
| Cyclopentanone                            | 75.84                                          | 0.1211                      |
| Cyclopentene                              | 15.61                                          | 0.1097                      |
| Cyclopropane                              | 8.293                                          | 0.07420                     |
| <i>p</i> -Cymene                          | 43.65                                          | 0.2386                      |
| Decane                                    | 52.88                                          | 0.3051                      |
| Decanenitrile                             | 34.71                                          | 0.1988                      |
| 1-Decanol                                 | 57.45                                          | 0.2971                      |
| 1-Decene                                  | 49.96                                          | 0.2888                      |
| Deuterium (normal)                        | 0.2583                                         | 0.02397                     |
| Deuterium oxide                           | 5.584                                          | 0.03090                     |
| Diborane (B <sub>2</sub> H <sub>6</sub> ) | 6.048                                          | 0.07437                     |
| Dibromodifluoromethane                    | 15.69                                          | 0.1186                      |
| 1,2-Dibromoethane                         | 13.98                                          | 0.08664                     |
| 1,2-Dibromotetrafluoroethane              | 20.45                                          | 0.1494                      |
| Dibutylamine                              | 34.61                                          | 0.2030                      |
| Dibutyl ether                             | 33.06                                          | 0.2017                      |
| Dibutyl sulfide                           | 49.3                                           | 0.2702                      |
| 1,2-Dichlorobenzene                       | 34.59                                          | 0.1767                      |
| 1,3-Dichlorobenzene                       | 35.44                                          | 0.1846                      |
| 1,4-Dichlorobenzene                       | 34.64                                          | 0.1802                      |
| Dichlorodifluoromethane                   | 10.45                                          | 0.09672                     |
| Dichlorodifluorosilane                    | 11.34                                          | 0.1095                      |
| 1,1-Dichloroethane                        | 15.73                                          | 0.1072                      |
| 1,2-Dichloroethane                        | 17.0                                           | 0.108                       |
| 1,1-Dichloroethylene                      | 13.74                                          | 0.09893                     |
| <i>trans</i> -1,2-Dichloroethylene        | 13.63                                          | 0.09573                     |
| Dichlorofluoromethane                     | 11.48                                          | 0.09060                     |
| Dichloromethane                           | 12.44                                          | 0.08689                     |
| 1,2-Dichloropropane                       | 21.62                                          | 0.1335                      |
| Dichlorosilane                            | 12.59                                          | 0.09992                     |
| 1,1-Dichlorotetrafluoroethane             | 15.49                                          | 0.1318                      |
| 1,2-Dichlorotetrafluoroethane             | 15.72                                          | 0.1338                      |
| Dideuterium oxide                         | 5.535                                          | 0.03062                     |
| Diethanolamine                            | 45.61                                          | 0.2273                      |
| Diethylamine                              | 19.40                                          | 0.1383                      |
| 1,4-Diethylbenzene                        | 45.03                                          | 0.2439                      |
| Diethylene glycol                         | 29.02                                          | 0.1519                      |
| Diethyl ether                             | 17.46                                          | 0.1333                      |
| 3,3-Diethylhexane                         | 47.69                                          | 0.2707                      |
| 3,4-Diethylhexane                         | 47.93                                          | 0.2760                      |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                              | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|----------------------------------------|--------------------------------------------------------|-------------------------------------|
| 3,3-Diethyl-2-methylpentane            | 47.20                                                  | 0.2629                              |
| 3,3-Diethylpentane                     | 40.64                                                  | 0.2374                              |
| Diethyl sulfide                        | 22.85                                                  | 0.1462                              |
| Difluoroamine                          | 5.028                                                  | 0.04446                             |
| <i>cis</i> -Difluorodiazine            | 3.043                                                  | 0.03987                             |
| <i>trans</i> -Difluorodiazine          | 3.539                                                  | 0.04851                             |
| 1,1-Difluoroethane                     | 9.691                                                  | 0.08931                             |
| 1,1-Difluoroethylene                   | 6.000                                                  | 0.07058                             |
| Difluoromethane                        | 6.184                                                  | 0.06268                             |
| Dihexyl ether                          | 69.17                                                  | 0.3752                              |
| Dihydrogen disulfide                   | 16.15                                                  | 0.1006                              |
| Diisopropyl ether                      | 25.26                                                  | 0.1836                              |
| Dimethoxyethane                        | 21.65                                                  | 0.1439                              |
| Dimethoxymethane                       | 17.28                                                  | 0.1195                              |
| <i>N,N</i> -Dimethoxyacetamide         | 30.19                                                  | 0.1689                              |
| Dimethylamine                          | 10.44                                                  | 0.08510                             |
| <i>N,N</i> -Dimethylaniline            | 37.92                                                  | 0.1967                              |
| 2,2-Dimethylbutane                     | 22.55                                                  | 0.1644                              |
| 2,3-Dimethylbutane                     | 23.29                                                  | 0.1660                              |
| 2,3-Dimethyl-1-butene                  | 22.59                                                  | 0.2566                              |
| 3,3-Dimethyl-1-butene                  | 21.55                                                  | 0.1567                              |
| 2,3-Dimethyl-2-butene                  | 23.83                                                  | 0.1621                              |
| 1,1-Dimethylcyclohexane                | 34.30                                                  | 0.2068                              |
| <i>cis</i> -1,2-Dimethylcyclohexane    | 36.44                                                  | 0.2143                              |
| <i>trans</i> -1,2-Dimethylcyclohexane  | 34.89                                                  | 0.2086                              |
| <i>cis</i> -1,3-Dimethylcyclohexane    | 34.30                                                  | 0.2068                              |
| <i>trans</i> -1,3-Dimethylcyclohexane  | 35.11                                                  | 0.2093                              |
| <i>cis</i> -1,4-Dimethylcyclohexane    | 35.47                                                  | 0.2114                              |
| <i>trans</i> -1,4-Dimethylcyclohexane  | 34.54                                                  | 0.2086                              |
| 1,1-Dimethylcyclopentane               | 25.37                                                  | 0.1653                              |
| <i>cis</i> -1,2-Dimethylcyclopentane   | 27.04                                                  | 0.1706                              |
| <i>trans</i> -1,2-Dimethylcyclopentane | 25.67                                                  | 0.1663                              |
| Dimethyl ether                         | 8.690                                                  | 0.07742                             |
| <i>N,N</i> -Dimethylformamide          | 23.57                                                  | 0.1293                              |
| 2,2-Dimethylheptane                    | 41.29                                                  | 0.2551                              |
| 2,2-Dimethylhexane                     | 34.87                                                  | 0.2260                              |
| 2,3-Dimethylhexane                     | 35.24                                                  | 0.2228                              |
| 2,4-Dimethylhexane                     | 34.97                                                  | 0.2251                              |
| 2,5-Dimethylhexane                     | 35.49                                                  | 0.2299                              |
| 3,3-Dimethylhexane                     | 34.72                                                  | 0.2201                              |
| 3,4-Dimethylhexane                     | 35.06                                                  | 0.2196                              |
| 1,1-Dimethylhydrazine                  | 14.69                                                  | 0.1001                              |
| 2,4-Dimethyl-3-isopentane              | 47.05                                                  | 0.2729                              |
| Dimethyl oxalate                       | 28.97                                                  | 0.1644                              |
| 2,2-Dimethylpentane                    | 28.49                                                  | 0.1951                              |
| 2,3-Dimethylpentane                    | 28.96                                                  | 0.1921                              |
| 2,4-Dimethylpentane                    | 28.79                                                  | 0.1974                              |
| 3,3-Dimethylpentane                    | 28.48                                                  | 0.1892                              |
| 2,3-Dimethylphenol                     | 31.35                                                  | 0.1545                              |
| 2,4-Dimethylphenol                     | 33.49                                                  | 0.1687                              |
| 2,5-Dimethylphenol                     | 29.99                                                  | 0.1512                              |
| 2,6-Dimethylphenol                     | 33.64                                                  | 0.1710                              |
| 3,4-Dimethylphenol                     | 31.32                                                  | 0.1529                              |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                           | $a$ , L <sup>2</sup> · bar · mol <sup>-2</sup> | $b$ , L · mol <sup>-1</sup> |
|-------------------------------------|------------------------------------------------|-----------------------------|
| 3,5-Dimethylphenol                  | 40.92                                          | 0.2037                      |
| 2,2-Dimethylpropane                 | 17.17                                          | 0.1410                      |
| 2,3-Dimethylpropane                 | 23.13                                          | 0.1669                      |
| 2,2-Dimethyl-1-propanol             | 22.25                                          | 0.1444                      |
| Dimethyl sulfide                    | 13.34                                          | 0.09453                     |
| <i>N,N</i> -Dimethyl-1,2-toluidine  | 41.71                                          | 0.2225                      |
| 1,4-Dioxane                         | 19.29                                          | 0.1171                      |
| Diphenyl ether                      | 54.61                                          | 0.2538                      |
| Diphenylmethane                     | 60.46                                          | 0.2798                      |
| Dipropylamine                       | 24.82                                          | 0.1591                      |
| Dipropyl ether                      | 27.12                                          | 0.1821                      |
| Dodecafluorocyclohexane             | 25.09                                          | 0.1955                      |
| Dodecafluoropentane                 | 25.58                                          | 0.2161                      |
| Dodecane                            | 69.14                                          | 0.3741                      |
| 1-Dodecanol                         | 72.69                                          | 0.3598                      |
| 1-Dodecene                          | 68.17                                          | 0.3694                      |
| Ethane                              | 5.570                                          | 0.06499                     |
| 1,2-Ethanediamine                   | 16.30                                          | 0.09796                     |
| Ethanethiol                         | 13.23                                          | 0.09447                     |
| Ethanol                             | 12.56                                          | 0.08710                     |
| Ethoxybenzene                       | 35.70                                          | 0.1996                      |
| Ethyl acetate                       | 20.57                                          | 0.1401                      |
| Ethyl acrylate                      | 23.70                                          | 0.1530                      |
| Ethylamine                          | 10.79                                          | 0.08433                     |
| Ethylbenzene                        | 30.86                                          | 0.1782                      |
| Ethyl benzoate                      | 43.73                                          | 0.2236                      |
| Ethyl butanoate                     | 30.53                                          | 0.1922                      |
| Ethylcyclohexane                    | 35.70                                          | 0.2089                      |
| Ethylcyclopentane                   | 27.90                                          | 0.1746                      |
| 3-Ethyl-2,2-dimethylhexane          | 47.24                                          | 0.2752                      |
| 4-Ethyl-2,2-dimethylhexane          | 46.45                                          | 0.2784                      |
| 3-Ethyl-2,3-dimethylhexane          | 47.35                                          | 0.2692                      |
| 4-Ethyl-2,3-dimethylhexane          | 47.49                                          | 0.2742                      |
| 3-Ethyl-2,4-dimethylhexane          | 47.31                                          | 0.2736                      |
| 4-Ethyl-2,4-dimethylhexane          | 45.52                                          | 0.2613                      |
| 3-Ethyl-2,5-dimethylhexane          | 47.42                                          | 0.2800                      |
| 3-Ethyl-3,4-dimethylhexane          | 47.00                                          | 0.2682                      |
| Ethylene                            | 4.612                                          | 0.05821                     |
| Ethylene glycol dimethyl ether      | 21.65                                          | 0.1439                      |
| Ethylene glycol ethyl ether acetate | 33.97                                          | 0.05594                     |
| Ethylene oxide                      | 8.922                                          | 0.06779                     |
| Ethyl formate                       | 15.91                                          | 0.1115                      |
| 3-Ethylhexane                       | 35.76                                          | 0.2253                      |
| Ethyl mercaptan                     | 11.24                                          | 0.08098                     |
| 2-Ethyl-1-methylbenzene             | 40.66                                          | 0.2226                      |
| 3-Ethyl-1-methylbenzene             | 41.67                                          | 0.2331                      |
| 4-Ethyl-1-methylbenzene             | 40.63                                          | 0.2262                      |
| 1-Ethyl-1-methylcyclopentane        | 34.18                                          | 0.2058                      |
| Ethyl methyl ether                  | 12.70                                          | 0.1034                      |
| 3-Ethyl-2-methylheptane             | 48.81                                          | 0.2847                      |
| Ethyl methyl ketone                 | 20.13                                          | 0.1340                      |
| 3-Ethyl-2-methylpentane             | 34.74                                          | 0.2183                      |
| 3-Ethyl-2-methylpentane             | 34.53                                          | 0.2134                      |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                | $a$ , L <sup>2</sup> · bar · mol <sup>-2</sup> | $b$ , L · mol <sup>-1</sup> |
|--------------------------|------------------------------------------------|-----------------------------|
| Ethyl 2-methylpropanoate | 29.05                                          | 0.1872                      |
| Ethyl methyl sulfide     | 19.45                                          | 0.1300                      |
| 3-Ethylpentane           | 29.49                                          | 0.1944                      |
| Ethyl phenyl ether       | 35.16                                          | 0.1963                      |
| Ethyl propanoate         | 25.86                                          | 0.1688                      |
| Ethyl propyl ether       | 22.45                                          | 0.1600                      |
| <i>m</i> -Ethyltoluene   | 41.73                                          | 0.2334                      |
| <i>o</i> -Ethyltoluene   | 40.67                                          | 0.2226                      |
| <i>p</i> -Ethyltoluene   | 40.63                                          | 0.2262                      |
| Ethyl vinyl ether        | 16.17                                          | 0.1213                      |
| Fluorine                 | 1.171                                          | 0.02896                     |
| Fluorobenzene            | 20.10                                          | 0.1279                      |
| Fluoroethane             | 8.170                                          | 0.07758                     |
| Fluoroethylene           | 5.984                                          | 0.06504                     |
| Fluoromethane            | 5.009                                          | 0.05617                     |
| Formaldehyde             | 7.356                                          | 0.06425                     |
| Furan                    | 12.74                                          | 0.0926                      |
| 2-Furaldehyde (furfural) | 22.23                                          | 0.1182                      |
| Germanium tetrachloride  | 23.12                                          | 0.1489                      |
| Germanium tetrahydride   | 5.743                                          | 0.06555                     |
| Glycerol                 | 22.98                                          | 0.07037                     |
| Hafnium tetrachloride    | 26.01                                          | 0.1282                      |
| Helium (equilibrium)     | 0.0346                                         | 0.02356                     |
| Heptane                  | 30.89                                          | 0.2038                      |
| 1-Heptanol               | 37.22                                          | 0.2097                      |
| 2-Heptanol               | 35.72                                          | 0.2093                      |
| 2-Heptanone              | 31.78                                          | 0.1850                      |
| 1-Heptene                | 28.82                                          | 0.09400                     |
| Hexadecafluoroheptane    | 40.58                                          | 0.3046                      |
| 1,5-Hexadiene            | 21.79                                          | 0.1532                      |
| Hexafluoroacetone        | 12.66                                          | 0.1264                      |
| Hexafluorobenzene        | 26.63                                          | 0.1641                      |
| Hexane                   | 24.97                                          | 0.1753                      |
| Hexanenitrile            | 35.50                                          | 0.1996                      |
| Hexanoic acid            | 39.94                                          | 0.2150                      |
| 1-Hexanol                | 31.35                                          | 0.1829                      |
| 2-Hexanol                | 30.25                                          | 0.1840                      |
| 3-Hexanol                | 29.44                                          | 0.1803                      |
| 2-Hexanone               | 30.27                                          | 0.1837                      |
| 3-Hexanone               | 29.84                                          | 0.1824                      |
| 1-Hexene                 | 23.12                                          | 0.1634                      |
| <i>cis</i> -2-Hexene     | 23.86                                          | 0.1641                      |
| <i>trans</i> -2-Hexene   | 23.75                                          | 0.1640                      |
| <i>cis</i> -3-Hexene     | 23.77                                          | 0.1638                      |
| <i>trans</i> -3-Hexene   | 24.25                                          | 0.1663                      |
| Hexylcyclopentane        | 59.38                                          | 0.3206                      |
| Hydrazine                | 8.46                                           | 0.0462                      |
| Hydrogen (normal)        | 0.2484                                         | 0.02651                     |
| Hydrogen bromide         | 4.500                                          | 0.04415                     |
| Hydrogen chloride        | 3.700                                          | 0.04061                     |
| Hydrogen cyanide         | 11.29                                          | 0.08806                     |
| Hydrogen deuteride       | 0.2527                                         | 0.02516                     |
| Hydrogen fluoride        | 9.565                                          | 0.0739                      |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                   | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|-----------------------------|--------------------------------------------------------|-------------------------------------|
| Hydrogen iodide             | 6.309                                                  | 0.05303                             |
| Hydrogen selenide           | 5.523                                                  | 0.0479                              |
| Hydrogen sulfide            | 4.544                                                  | 0.04339                             |
| Indane                      | 34.63                                                  | 0.1802                              |
| Iodobenzene                 | 33.54                                                  | 0.1658                              |
| Iodomethane                 | 12.34                                                  | 0.08327                             |
| Isobutyl acetate            | 29.05                                                  | 0.1845                              |
| Isobutylamine               | 19.30                                                  | 0.1325                              |
| Isobutylbenzene             | 40.40                                                  | 0.2215                              |
| Isobutylcyclohexane         | 40.39                                                  | 0.2195                              |
| Isobutyl formate            | 22.82                                                  | 0.1476                              |
| Isopropylamine              | 14.30                                                  | 0.1080                              |
| Isopropylbenzene            | 36.20                                                  | 0.2044                              |
| Isopropylcyclohexane        | 42.06                                                  | 0.2342                              |
| Isopropylcyclopentane       | 35.11                                                  | 0.2082                              |
| 4-Isopropylheptane          | 48.28                                                  | 0.2832                              |
| 2-Isopropyl-1-methylbenzene | 45.14                                                  | 0.2401                              |
| 3-Isopropyl-1-methylbenzene | 44.00                                                  | 0.2354                              |
| 4-Isopropyl-1-methylbenzene | 43.94                                                  | 0.2398                              |
| 3-Isopropyl-2-methylhexane  | 50.93                                                  | 0.2870                              |
| Ketene                      | 19.1                                                   | 0.1044                              |
| Krypton                     | 2.325                                                  | 0.0396                              |
| Mercury                     | 5.193                                                  | 0.01057                             |
| Methane                     | 2.300                                                  | 0.04301                             |
| Methanethiol                | 8.911                                                  | 0.06756                             |
| Methanol                    | 9.472                                                  | 0.06584                             |
| Methoxybenzoate             | 28.60                                                  | 0.1579                              |
| Methyl acetate              | 15.75                                                  | 0.1108                              |
| Methyl acrylate             | 19.67                                                  | 0.1308                              |
| Methylamine                 | 7.106                                                  | 0.05879                             |
| 2-Methyl-1,3-butadiene      | 17.74                                                  | 0.1307                              |
| 3-Methyl-1,3-butadiene      | 17.46                                                  | 0.1245                              |
| 2-Methylbutane              | 18.29                                                  | 0.1415                              |
| Methyl butanoate            | 25.83                                                  | 0.1661                              |
| 3-Methylbutanoic acid       | 33.94                                                  | 0.1923                              |
| 2-Methyl-1-butanol          | 24.51                                                  | 0.1518                              |
| 3-Methyl-1-butanol          | 24.72                                                  | 0.1526                              |
| 2-Methyl-2-butanol          | 23.24                                                  | 0.1523                              |
| 3-Methyl-2-butanol          | 23.30                                                  | 0.1493                              |
| 3-Methyl-2-butanone         | 23.20                                                  | 0.1494                              |
| 2-Methyl-1-butene           | 16.9                                                   | 0.129                               |
| 3-Methyl-1-butene           | 18.08                                                  | 0.1405                              |
| 2-Methyl-2-butene           | 17.26                                                  | 0.1279                              |
| Methylcyclohexane           | 27.51                                                  | 0.1713                              |
| Methylcyclopentane          | 21.87                                                  | 0.1463                              |
| N-Methylethylamine          | 19.39                                                  | 0.1391                              |
| Methyl formate              | 11.54                                                  | 0.08406                             |
| 2-Methylfuran               | 14.67                                                  | 0.1160                              |
| 2-Methylheptane             | 36.78                                                  | 0.2342                              |
| 3-Methylheptane             | 36.40                                                  | 0.2301                              |
| 4-Methylheptane             | 36.21                                                  | 0.2297                              |
| 2-Methylhexane              | 30.01                                                  | 0.2016                              |
| 3-Methylhexane              | 29.70                                                  | 0.1977                              |



**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                           | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|-------------------------------------|--------------------------------------------------------|-------------------------------------|
| Methylhydrazine                     | 11.67                                                  | 0.07334                             |
| Methyl isobutanoate                 | 24.87                                                  | 0.1639                              |
| Methyl isocyanate                   | 12.6                                                   | 0.09161                             |
| 1-Methyl-2-isopropylbenzene         | 42.7                                                   | 0.234                               |
| 1-Methyl-4-isopropylbenzene         | 45.27                                                  | 0.2478                              |
| Methyl 2-methylpropanoate           | 24.50                                                  | 0.163 7                             |
| 2-Methyloctane                      | 43.50                                                  | 0.2641                              |
| 2-Methylpentane                     | 23.83                                                  | 0.1707                              |
| 3-Methylpentane                     | 23.75                                                  | 0.1677                              |
| 2-Methyl-2,4-pentanediol            | 39.05                                                  | 0.2054                              |
| Methyl pentanoate                   | 29.39                                                  | 0.1847                              |
| 2-Methyl-3-pentanol                 | 27.96                                                  | 0.1730                              |
| 3-Methyl-3-pentanol                 | 27.45                                                  | 0.1699                              |
| 4-Methyl-2-pentanol                 | 22.38                                                  | 0.1388                              |
| 4-Methyl-2-pentanone                | 29.08                                                  | 0.1815                              |
| 2-Methyl-2-pentene                  | 23.86                                                  | 0.1641                              |
| <i>cis</i> -3-Methyl-2-pentene      | 23.86                                                  | 0.1641                              |
| <i>trans</i> -3-Methyl-2-pentene    | 24.60                                                  | 0.1656                              |
| <i>cis</i> -4-Methyl-2-pentene      | 23.03                                                  | 0.1675                              |
| <i>trans</i> -4-Methyl-2-pentene    | 23.32                                                  | 0.1685                              |
| 2-Methylpropanal                    | 18.49                                                  | 0.1285                              |
| 2-Methyl-1-propanamine              | 19.30                                                  | 0.1325                              |
| 2-Methylpropane (isobutane)         | 13.36                                                  | 0.1168                              |
| Methyl propanoate                   | 20.51                                                  | 0.1377                              |
| 2-Methylpropanoic acid              | 28.9                                                   | 0.170                               |
| 2-Methyl-1-propanol                 | 20.35                                                  | 0.1324                              |
| 2-Methyl-2-propanol                 | 18.81                                                  | 0.1324                              |
| 2-Methylpropene                     | 12.73                                                  | 0.1086                              |
| 2-Methylpropyl acetate              | 29.05                                                  | 0.1845                              |
| 2-Methylpropyl formate              | 22.54                                                  | 0.1476                              |
| 2-Methylpyridine                    | 24.45                                                  | 0.1403                              |
| 3-Methylpyridine                    | 27.08                                                  | 0.1496                              |
| 4-Methylpyridine                    | 25.89                                                  | 0.1428                              |
| 1-Methylstyrene                     | 36.69                                                  | 0.1999                              |
| 2-Methyltetrahydrofuran             | 22.37                                                  | 0.1484                              |
| 2-Methylthiophene                   | 22.10                                                  | 0.1299                              |
| 3-Methylthiophene                   | 21.98                                                  | 0.1282                              |
| Methyl vinyl ether                  | 11.65                                                  | 0.09520                             |
| Morpholine                          | 20.36                                                  | 0.1174                              |
| Naphthalene                         | 40.32                                                  | 0.1920                              |
| Neon                                | 0.208                                                  | 0.01709                             |
| Niobium pentafluoride               | 25.22                                                  | 0.1220                              |
| Nitric oxide (NO)                   | 1.46                                                   | 0.0289                              |
| Nitroethane                         | 24.13                                                  | 0.1544                              |
| Nitrogen-14                         | 15.18                                                  | 0.1288                              |
| Nitrogen chloride difluoride        | 6.447                                                  | 0.06089                             |
| Nitrogen dioxide (NO <sub>2</sub> ) | 5.36                                                   | 0.0443                              |
| Nitrogen trifluoride                | 3.58                                                   | 0.05364                             |
| Nitrous oxide (N <sub>2</sub> O)    | 3.852                                                  | 0.04435                             |
| Nitromethane                        | 17.18                                                  | 0.1041                              |
| Nitrosyl chloride                   | 6.191                                                  | 0.05014                             |
| Nonane                              | 45.11                                                  | 0.2702                              |
| 1-Nonanol                           | 50.00                                                  | 0.2634                              |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                                      | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|------------------------------------------------|--------------------------------------------------------|-------------------------------------|
| 1-Nonene                                       | 43.68                                                  | 0.2629                              |
| Octadecafluorooctane                           | 44.27                                                  | 0.3143                              |
| Octafluorocyclobutane                          | 15.81                                                  | 0.1450                              |
| Octafluoropropane                              | 12.96                                                  | 0.1338                              |
| Octamethylcyclotetrasiloxane                   | 75.30                                                  | 0.4579                              |
| Octane                                         | 37.86                                                  | 0.2370                              |
| 1-Octanol                                      | 44.71                                                  | 0.2371                              |
| 2-Octanol                                      | 41.98                                                  | 0.2376                              |
| 1-Octene                                       | 35.01                                                  | 0.2227                              |
| <i>cis</i> -2-Octene                           | 35.42                                                  | 0.2176                              |
| Osmium tetroxide                               | 2.79                                                   | 0.2447                              |
| Oxygen                                         | 1.382                                                  | 0.03186                             |
| Oxygen difluoride                              | 2.726                                                  | 0.04516                             |
| Ozone                                          | 3.570                                                  | 0.04977                             |
| Pentadecane                                    | 95.91                                                  | 0.4834                              |
| 1-Pentadecene                                  | 99.00                                                  | 0.5011                              |
| 1,2-Pentadiene                                 | 18.13                                                  | 0.1284                              |
| <i>cis</i> -1,3-Pentadiene                     | 17.98                                                  | 0.1292                              |
| 1,4-Pentadiene                                 | 17.58                                                  | 0.1311                              |
| Pentafluorobenzene                             | 23.45                                                  | 0.1571                              |
| 2,2,3,3,4-Pentamethylpentane                   | 46.85                                                  | 0.2593                              |
| 2,2,3,4,4-Pentamethylpentane                   | 47.82                                                  | 0.2716                              |
| Pentanal                                       | 25.21                                                  | 0.1622                              |
| Pentane                                        | 19.13                                                  | 0.1449                              |
| Pentanenitrile                                 | 34.16                                                  | 0.1772                              |
| Pentanoic acid                                 | 33.68                                                  | 0.1867                              |
| 1-Pentanol                                     | 25.81                                                  | 0.1572                              |
| 2-Pentanol                                     | 24.89                                                  | 0.1585                              |
| 2-Pentanone                                    | 24.85                                                  | 0.1578                              |
| 3-Pentanone                                    | 24.65                                                  | 0.1565                              |
| 1-Pentene                                      | 17.86                                                  | 0.1370                              |
| <i>cis</i> -2-Pentene                          | 17.83                                                  | 0.1338                              |
| <i>trans</i> -2-Pentene                        | 18.30                                                  | 0.1391                              |
| Pentylbenzene                                  | 51.85                                                  | 0.2718                              |
| Pentyl formate                                 | 27.97                                                  | 0.1730                              |
| 1-Pentyne                                      | 17.53                                                  | 0.1266                              |
| Perchloryl fluoride ( $\text{ClO}_3\text{F}$ ) | 7.371                                                  | 0.07130                             |
| Phenol                                         | 22.93                                                  | 0.1177                              |
| Phosgene                                       | 10.65                                                  | 0.08340                             |
| Phosphine                                      | 4.693                                                  | 0.05155                             |
| Phosphonium chloride                           | 4.111                                                  | 0.04545                             |
| Phosphorus                                     | 53.6                                                   | 0.157                               |
| Phosphorus chloride difluoride                 | 8.47                                                   | 0.0833                              |
| Phosphorus dichloride fluoride                 | 12.50                                                  | 0.0962                              |
| Phosphorus trifluoride                         | 4.954                                                  | 0.06510                             |
| Phosphoryl chloride difluoride                 | 11.90                                                  | 0.1001                              |
| Phosphoryl trifluoride                         | 8.26                                                   | 0.0849                              |
| Piperidine                                     | 20.84                                                  | 0.1250                              |
| Propadiene                                     | 8.23                                                   | 0.0747                              |
| Propanal                                       | 14.08                                                  | 0.0995                              |
| Propane                                        | 9.385                                                  | 0.09044                             |
| 1,2-Propanediol                                | 18.74                                                  | 0.1068                              |
| 1,3-Propanediol                                | 21.11                                                  | 0.1143                              |

TABLE 5.29 Van der Waals' Constants for Gases (Continued)

| Substance                                             | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|-------------------------------------------------------|--------------------------------------------------------|-------------------------------------|
| Propanenitrile                                        | 21.57                                                  | 0.1369                              |
| Propanoic acid                                        | 23.49                                                  | 0.1386                              |
| 1-Propanol                                            | 16.26                                                  | 0.1080                              |
| 2-Propanol                                            | 15.82                                                  | 0.1109                              |
| 2-Propenal                                            | 14.44                                                  | 0.1017                              |
| Propene                                               | 8.411                                                  | 0.08211                             |
| Propyl acetate                                        | 26.23                                                  | 0.1700                              |
| Propylamine                                           | 15.26                                                  | 0.1095                              |
| Propylbenzene                                         | 37.14                                                  | 0.2073                              |
| Propylcyclopentane                                    | 38.80                                                  | 0.2189                              |
| Propylcyclohexane                                     | 38.59                                                  | 0.2255                              |
| Propylene oxide                                       | 13.78                                                  | 0.1019                              |
| Propyl formate                                        | 20.79                                                  | 0.1377                              |
| Propyne                                               | 8.40                                                   | 0.0744                              |
| Pyridine                                              | 19.77                                                  | 0.1136                              |
| Pyrrrole                                              | 18.82                                                  | 0.1049                              |
| Pyrrolidine                                           | 16.84                                                  | 0.1056                              |
| Quinoline                                             | 36.70                                                  | 0.1672                              |
| Radon                                                 | 6.601                                                  | 0.06239                             |
| Selenium                                              | 33.4                                                   | 0.0675                              |
| Silicon chloride trifluoride                          | 7.95                                                   | 0.0921                              |
| Silicon tetrachloride                                 | 20.96                                                  | 0.1470                              |
| Silicon tetrafluoride                                 | 5.259                                                  | 0.072361                            |
| Silicon tetrahydride (silane)                         | 4.30                                                   | 0.0579                              |
| Styrene                                               | 32.15                                                  | 0.1799                              |
| Sulfur (S)                                            | 24.3                                                   | 0.0660                              |
| Sulfur dioxide                                        | 6.714                                                  | 0.05636                             |
| Sulfur hexafluoride (SF <sub>6</sub> )                | 7.857                                                  | 0.08786                             |
| Sulfur trioxide                                       | 8.57                                                   | 0.0622                              |
| 1,1,2,2-Tetrachlorodifluoroethane                     | 25.74                                                  | 0.1665                              |
| Tetrachloroethylene                                   | 24.98                                                  | 0.1435                              |
| Tetrachloromethane                                    | 20.01                                                  | 0.1281                              |
| Tetradecafluorohexane                                 | 30.75                                                  | 0.2448                              |
| Tetradecafluoromethylcyclohexane                      | 29.66                                                  | 0.2171                              |
| 1-Tetradecanol                                        | 89.91                                                  | 0.4289                              |
| Tetraethylsilane                                      | 40.85                                                  | 0.2411                              |
| Tetrafluoroethylene                                   | 6.954                                                  | 0.08085                             |
| Tetrafluorohydrazine (N <sub>2</sub> F <sub>4</sub> ) | 7.426                                                  | 0.08564                             |
| Tetrafluoromethane                                    | 4.040                                                  | 0.06325                             |
| Tetrahydrofuran                                       | 16.39                                                  | 0.1082                              |
| Tetrahydropyran                                       | 20.02                                                  | 0.1247                              |
| 1,2,4,5-Tetramethylbenzene                            | 45.8                                                   | 0.2422                              |
| 2,2,3,3-Tetramethylbutane                             | 32.76                                                  | 0.2056                              |
| 2,2,3,3-Tetramethylhexane                             | 45.11                                                  | 0.2580                              |
| 2,2,3,4-Tetramethylhexane                             | 47.36                                                  | 0.2721                              |
| 2,2,3,5-Tetramethylhexane                             | 46.45                                                  | 0.2753                              |
| 2,2,4,4-Tetramethylhexane                             | 48.26                                                  | 0.2819                              |
| 2,2,4,5-Tetramethylhexane                             | 47.05                                                  | 0.2802                              |
| 2,2,5,5-Tetramethylhexane                             | 45.03                                                  | 0.2760                              |
| 2,3,3,4-Tetramethylhexane                             | 47.13                                                  | 0.2653                              |
| 2,3,3,5-Tetramethylhexane                             | 46.79                                                  | 0.2733                              |
| 2,3,4,4-Tetramethylhexane                             | 47.32                                                  | 0.2691                              |
| 2,3,4,5-Tetramethylhexane                             | 46.86                                                  | 0.2723                              |

**TABLE 5.29** Van der Waals' Constants for Gases (*Continued*)

| Substance                      | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|--------------------------------|--------------------------------------------------------|-------------------------------------|
| 3,3,4,4-Tetramethylhexane      | 47.46                                                  | 0.2615                              |
| 2,2,3,3-Tetramethylpentane     | 39.29                                                  | 0.2304                              |
| 2,2,3,4-Tetramethylpentane     | 39.37                                                  | 0.2367                              |
| 2,2,4,4-Tetramethylpentane     | 38.76                                                  | 0.2403                              |
| 2,3,3,4-Tetramethylpentane     | 39.65                                                  | 0.2325                              |
| Tetramethylsilane              | 20.81                                                  | 0.1653                              |
| Thiophene                      | 17.21                                                  | 0.1058                              |
| Tin(IV) chloride               | 27.25                                                  | 0.1641                              |
| Titanium(IV) chloride          | 25.47                                                  | 0.1423                              |
| Toluene                        | 24.89                                                  | 0.1499                              |
| 1,2-Toluidine                  | 33.36                                                  | 0.1681                              |
| 1,3-Toluidine                  | 34.06                                                  | 0.1717                              |
| 1,4-Toluidine                  | 31.74                                                  | 0.1602                              |
| Tributoxyborane                | 81.34                                                  | 0.3891                              |
| Tributylamine                  | 65.31                                                  | 0.3645                              |
| 1,1,1-Trichloroethane          | 20.14                                                  | 0.1317                              |
| 1,1,2-Trichloroethane          | 25.47                                                  | 0.1508                              |
| Trichloroethylene              | 17.21                                                  | 0.1127                              |
| Trichlorofluoromethane         | 14.68                                                  | 0.1111                              |
| Trichlorofluorosilane          | 15.67                                                  | 0.1277                              |
| Trichloromethane               | 15.34                                                  | 0.1019                              |
| Trichloromethylsilane          | 23.77                                                  | 0.1638                              |
| 1,2,3-Trichloropropane         | 31.29                                                  | 0.1713                              |
| 1,1,2-Trichlorotrifluoroethane | 20.25                                                  | 0.1481                              |
| 1,2,2-Trichlorotrifluoroethane | 20.25                                                  | 0.1481                              |
| Tridecane                      | 79.09                                                  | 0.4176                              |
| 1-Tridecanol                   | 81.20                                                  | 0.3942                              |
| 1-Tridecene                    | 77.93                                                  | 0.4121                              |
| Tridecylcyclopentane           | 139.6                                                  | 0.6536                              |
| Triethanolamine                | 32.14                                                  | 0.3340                              |
| Triethylamine                  | 27.59                                                  | 0.1836                              |
| Trifluoroacetic acid           | 21.61                                                  | 0.1567                              |
| 1,1,1-Trifluoroethane          | 9.302                                                  | 0.09572                             |
| Trifluoromethane               | 5.378                                                  | 0.06403                             |
| Trimethylamine                 | 13.37                                                  | 0.1101                              |
| 1,2,3-Trimethylbenzene         | 37.28                                                  | 0.1999                              |
| 1,2,4-Trimethylbenzene         | 38.03                                                  | 0.2088                              |
| 1,3,5-Trimethylbenzene         | 37.87                                                  | 0.2118                              |
| 2,2,3-Trimethylbutane          | 27.86                                                  | 0.1869                              |
| 2,2,3-Trimethyl-1-butene       | 28.57                                                  | 0.1910                              |
| 1,1,2-Trimethylcyclopentane    | 33.31                                                  | 0.2048                              |
| 1,1,3-Trimethylcyclopentane    | 33.42                                                  | 0.2091                              |
| 2,2,3-Trimethylheptane         | 48.07                                                  | 0.2801                              |
| 2,2,4-Trimethylheptane         | 47.49                                                  | 0.2847                              |
| 2,3,4-Trimethylheptane         | 47.96                                                  | 0.2785                              |
| 3,3,4-Trimethylheptane         | 47.68                                                  | 0.2730                              |
| 2,2,3-Trimethylhexane          | 40.5                                                   | 0.2452                              |
| 2,2,4-Trimethylhexane          | 40.50                                                  | 0.2516                              |
| 2,2,5-Trimethylhexane          | 40.38                                                  | 0.2533                              |
| 2,2,3-Trimethylpentane         | 33.92                                                  | 0.2145                              |
| 2,2,4-Trimethylpentane         | 33.61                                                  | 0.2202                              |
| 2,3,3-Trimethylpentane         | 34.03                                                  | 0.2114                              |
| 2,3,4-Trimethylpentane         | 34.28                                                  | 0.2157                              |

TABLE 5.29 Van der Waals' Constants for Gases (Continued)

| Substance                               | $a, \text{L}^2 \cdot \text{bar} \cdot \text{mol}^{-2}$ | $b, \text{L} \cdot \text{mol}^{-1}$ |
|-----------------------------------------|--------------------------------------------------------|-------------------------------------|
| 2,2,4-Trimethyl-1,3-pentanediol         | 19.96                                                  | 0.2692                              |
| Tungsten(VI) fluoride ( $\text{WF}_6$ ) | 13.25                                                  | 0.1063                              |
| Undecane                                | 60.88                                                  | 0.3396                              |
| 1-Undecene                              | 59.17                                                  | 0.3310                              |
| Uranium(VI) fluoride ( $\text{UF}_6$ )  | 16.01                                                  | 0.1128                              |
| Vinyl acetate                           | 32.31                                                  | 0.2296                              |
| Vinyl chloride                          | 9.62                                                   | 0.07975                             |
| Vinyl fluoride                          | 5.98                                                   | 0.06502                             |
| Vinyl formate                           | 11.38                                                  | 0.08541                             |
| Xenon                                   | 4.192                                                  | 0.05156                             |
| Xenon difluoride                        | 12.46                                                  | 0.7037                              |
| Xenon tetrafluoride                     | 15.52                                                  | 0.09035                             |
| <i>m</i> -Xylene                        | 31.41                                                  | 0.1814                              |
| <i>o</i> -Xylene                        | 31.06                                                  | 0.1756                              |
| <i>p</i> -Xylene                        | 31.54                                                  | 0.1824                              |
| Water                                   | 5.537                                                  | 0.03052                             |
| Zirconium(IV) chloride                  | 30.59                                                  | 0.1401                              |

TABLE 5.30 Triple Points of Various Materials

| Substance                      | Triple point, K | Pressure, mmHg |
|--------------------------------|-----------------|----------------|
| Ammonia                        | 195.46          | 45.58          |
| Argon                          | 83.78           | 516            |
| Boron tribromide               | 226.67          |                |
| Bromine                        | 280.4           | 44.1           |
| Carbon dioxide                 | 216.65          |                |
| Cyclopropane                   | 145.59          |                |
| Deuterium oxide                | 276.97          |                |
| 1-Hexene                       | 133.39          |                |
| Hydrogen, normal               | 13.95           | 54             |
| Hydrogen, para                 | 13.81           |                |
| Hydrogen bromide               | 186.1           | ~232           |
| Hydrogen chloride              | 158.8           |                |
| Iodine heptafluoride           | 279.6           |                |
| Krypton                        | 115.95          | 548            |
| Methane                        | 90.67           | 87.60          |
| Methane- $d_1$                 | 90.40           | 84.52          |
| Methane- $d_2$                 | 90.14           | 81.80          |
| Methane- $d_3$                 | 89.94           | 80.12          |
| Methane- $d_4$                 | 89.79           | 79.13          |
| Molybdenum oxide tetrafluoride | 370.3           |                |
| Molybdenum pentafluoride       | 340             |                |
| Neon                           | 24.55           | 324            |
| Neptunium hexafluoride         | 328.25          | 758.0          |
| Niobium pentabromide           | 540.6           |                |
| Niobium pentachloride          | 476.5           |                |
| Nitrogen                       | 63.15           | 94             |
| 1-Octene                       | 171.45          |                |
| Oxygen                         | 54.34           |                |

**TABLE 5.30** Triple Points of Various Materials (*Continued*)

| Substance                      | Triple point, K | Pressure, mmHg |
|--------------------------------|-----------------|----------------|
| Phosphorus, white              | 863             | 32 760         |
| Plutonium hexafluoride         | 324.74          | 533.0          |
| Propene                        | 103.95          |                |
| Radon                          | 202             | ~500           |
| Rhenium dioxide trifluoride    | 363             |                |
| Rhenium heptafluoride          | 321.4           |                |
| Rhenium oxide pentafluoride    | 313.9           |                |
| Rhenium pentafluoride          | 321             |                |
| Succinonitrile (NIST standard) | 331.23          |                |
| Sulfur dioxide                 | 197.68          | 1.256          |
| Tantalum pentabromide          | 553             |                |
| Tantalum pentachloride         | 489.0           |                |
| Tungsten oxide tetrafluoride   | 377.8           |                |
| Uranium hexafluoride           | 337.20          | 1 139.6        |
| Water                          | 273.16          |                |
| Xenon                          | 161.37          | 612            |

### 5.9.1 Some Physical Chemistry Equations for Gases

A number of physical chemistry relationships, not enumerated in other sections (*see* Index), will be discussed in this section.

*Boyle's law* states that the volume of a given quantity of a gas varies inversely as the pressure, the temperature remaining constant. That is,

$$V = \frac{\text{constant}}{P} \quad \text{or} \quad PV = \text{constant}$$

A convenient form of the law, true strictly for ideal gases, is

$$P_1 V_1 = P_2 V_2$$

*Charles' law*, also known as *Gay-Lussac's law*, states that the volume of a given mass of gas varies directly as the absolute temperature if the pressure remains constant, that is,

$$\frac{V}{T} = \text{constant}$$

Combining the laws of Boyle and Charles into one expression gives

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

In terms of moles, *Avogadro's hypothesis* can be stated: The same volume is occupied by one mole of any gas at a given temperature and pressure. The number of molecules in one mole is known as the *Avogadro number constant*  $N_A$ .

The behavior of all gases that obey the laws of Boyle and Charles, and Avogadro's hypothesis, can be expressed by the ideal gas equation:

$$PV = nRT$$

where  $R$  is called the *gas constant* and  $n$  is the number of moles of gas. If pressure is written as force per unit area and the volume as area times length, then  $R$  has the dimensions of energy per degree per mole— $8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  or  $1.987 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ .

*Dalton's law of partial pressures* states that the total pressure exerted by a mixture of gases is equal to the sum of the pressures which each component would exert if placed separately into the container:

$$P_{\text{total}} = p_1 + p_2 + p_3 + \cdots$$

There are two ways to express the fraction which one gaseous component contributes to the total mixture: (1) the pressure fraction,  $p_i/P_{\text{total}}$ , and (2) the mole fraction,  $n_i/n_{\text{total}}$ .

### 5.9.1.1 Equations of State (PVT Relations for Real Gases)

1. *Virial equation* represents the experimental compressibility of a gas by an empirical equation of state:

$$PV = A_p + B_p P + C_p P^2 + \cdots$$

or

$$PV = A_v + B_v V + \frac{C_v}{V^2} + \cdots$$

where  $A, B, C, \dots$  are called the virial coefficients and are a function of the nature of the gas and the temperature.

2. *Van der Waals' equation*:

$$\left( P + \frac{an^2}{V^2} \right) (V - nb) = nRT$$

where the term  $an^2/V^2$  is the correction for intermolecular attraction among the gas molecules and the  $nb$  term is the correction for the volume occupied by the gas molecules. The constants  $a$  and  $b$  must be fitted for each gas from experimental data (Table 5.28); consequently the equation is semiempirical. The constants are related to the critical-point constants (Table 6.5) as follows:

$$a = 3P_c V_c^2$$

$$b = \frac{V_c}{3}$$

$$R = \frac{8P_c V_c}{3T_c}$$

Substitution into van der Waals' equation and rearrangement leads to only the terms  $P/P_c$ ,  $V/V_c$ , and  $T/T_c$ , which are called the reduced variables  $P_R$ ,  $V_R$ , and  $T_R$ . For 1 mole of gas,

$$\left( P_R + \frac{3}{V_R^2} \right) \left( V_R - \frac{1}{3} \right) = \frac{8}{3} T_R$$

3. *Berthelot's equation of state*, used by many thermodynamicists, is

$$PV = nRT \left[ 1 + \frac{9}{128} \frac{P T_c}{P_c T} \left( 1 - 6 \frac{T_c^2}{T^2} \right) \right]$$

This equation requires only knowledge of the critical temperature and pressure for its use and gives accurate results in the vicinity of room temperature for unassociated substances at moderate pressures.

### 5.9.1.2 Properties of Gas Molecules

**Vapor Density.** Substitution of the Antoine vapor-pressure equation for its equivalent  $\log P$  in the ideal gas equation gives

$$\log \rho_{\text{vap}} = \log M - \log R - \log (t + 273.15) + A - \frac{B}{t + C}$$

where  $\rho_{\text{vap}}$  is the vapor density in  $\text{g} \cdot \text{mL}^{-1}$  at  $t^\circ\text{C}$ ,  $M$  is the molecular weight,  $R$  is the gas constant, and  $A$ ,  $B$ , and  $C$  are the constants of the Antoine equation for vapor pressure. Since this equation is based on the ideal gas law, it is accurate only at temperatures at which the vapor of any specific compound follows this law. This condition prevails at reduced temperatures ( $T_R$ ) of about 0.5 K.

**Velocities of Molecules.** The mean square velocity of gas molecules is given by

$$\overline{u^2} = \frac{3kT}{m} = \frac{3RT}{M}$$

where  $k$  is Boltzmann's constant and  $m$  is the mass of the molecule.

The mean velocity is given by

$$\bar{u} = \left( \frac{8\overline{u^2}}{3\pi} \right)^{1/2}$$

**Viscosity.** On the assumption that molecules interact like hard spheres, the viscosity of a gas is

$$\eta = \left( \frac{5}{16\sigma^2} \right) \left( \frac{mkT}{\pi} \right)^{1/2}$$

where  $\sigma$  is the molecular diameter.

**Mean Free Path.** The mean free path of a gas molecule  $l$  and the mean time between collisions  $\tau$  are given by

$$l = \frac{m}{\pi\rho\sigma^2\sqrt{2}}$$

$$\tau = \frac{1}{\bar{u}} = \frac{4\eta}{5P}$$

**Graham's Law of Diffusion.** The rates at which gases diffuse under the same conditions of temperature and pressure are inversely proportional to the square roots of their densities:

$$\frac{r_1}{r_2} = \left( \frac{\rho_2}{\rho_1} \right)^{1/2}$$

Since  $\rho = MP/RT$  for an ideal gas, it follows that

$$\frac{r_1}{r_2} = \left( \frac{M_2}{M_1} \right)^{1/2}$$



*Henry's Law.* The solubility of a gas is directly proportional to the partial pressure exerted by the gas:

$$p_i = k\alpha_i$$

*Joule-Thompson Coefficient for Real Gases.* This expresses the change in temperature with respect to change in pressure at constant enthalpy:

$$\mu_\pi = \left( \frac{\partial T}{\partial P} \right)_H$$

---

# SECTION 6

---

## THERMODYNAMIC PROPERTIES

---

|              |                                                                                                                                  |              |
|--------------|----------------------------------------------------------------------------------------------------------------------------------|--------------|
| <b>6.1</b>   | <b>ENTHALPIES AND GIBBS ENERGIES OF FORMATION, ENTROPIES, AND HEAT CAPACITIES</b>                                                | <b>6.1</b>   |
| <b>6.1.1</b> | <b>Some Thermodynamic Relations</b>                                                                                              | <b>6.2</b>   |
| Table 6.1    | Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds                                  | 6.5          |
| Table 6.2    | Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds                    | 6.51         |
| Table 6.3    | Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds               | 6.81         |
| Table 6.4    | Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds | 6.124        |
| <b>6.2</b>   | <b>CRITICAL PHENOMENA</b>                                                                                                        | <b>6.142</b> |
| Table 6.5    | Critical Properties                                                                                                              | 6.143        |

---

### 6.1 ENTHALPIES AND GIBBS ENERGIES OF FORMATION, ENTROPIES, AND HEAT CAPACITIES

---

The tables in this section contain values of the enthalpy and Gibbs energy of formation, entropy, and heat capacity at 298.15 K (25°C). No values are given in these tables for metal alloys or other solid solutions, for fused salts, or for substances of undefined chemical composition.

The physical state of each substance is indicated in the column headed “State” as crystalline solid (c), liquid (lq), or gaseous (g). Solutions in water are listed as aqueous (aq).

The values of the thermodynamic properties of the pure substances given in these tables are, for the substances in their standard states, defined as follows: For a pure solid or liquid, the standard state is the substance in the condensed phase under a pressure of 1 atm (101 325 Pa). For a gas, the standard state is the hypothetical ideal gas at unit fugacity, in which state the enthalpy is that of the real gas at the same temperature and at zero pressure.

The values of  $\Delta_f H^\circ$  and  $\Delta_f G^\circ$  that are given in the tables represent the change in the appropriate thermodynamic quantity when one mole of the substance in its standard state is formed, isothermally at the indicated temperature, from the elements, each in its appropriate standard reference state. The standard reference state at 25°C for each element has been chosen to be the standard state that is thermodynamically stable at 25°C and 1 atm pressure. The standard reference states are indicated in the tables by the fact that the values of  $\Delta_f H^\circ$  and  $\Delta_f G^\circ$  are exactly zero.

The values of  $S^\circ$  represent the virtual or “thermal” entropy of the substance in the standard state at 298.15 K (25°C), omitting contributions from nuclear spins. Isotope mixing effects are also excluded except in the case of the  $^1\text{H}$ — $^2\text{H}$  system.

Solutions in water are designated as aqueous, and the concentration of the solution is expressed in terms of the number of moles of solvent associated with 1 mol of the solute. If no concentration is indicated, the solution is assumed to be dilute. The standard state for a solute in aqueous solution is taken as the hypothetical ideal solution of unit molality (indicated as std. state or ss). In this state

the partial molal enthalpy and the heat capacity of the solute are the same as in the infinitely dilute real solution.

For some tables the uncertainty of entries is indicated within parentheses immediately following the value; viz., an entry 34.5(4) implies  $34.5 \pm 0.4$  and an entry 34.5(12) implies  $34.5 \pm 1.2$ .

References: D. D. Wagman, et al., *The NBS Tables of Chemical Thermodynamic Properties*, in *J. Phys. Chem. Ref. Data*, **11: 2**, 1982; M. W. Chase, et al., *JANAF Thermochemical Tables*, 3rd ed., American Chemical Society and the American Institute of Physics, 1986 (supplements to JANAF appear in *J. Phys. Chem. Ref. Data*); Thermodynamic Research Center, *TRC Thermochemical Tables*, Texas A&M University, College Station, Texas; I. Barin and O. Knacke, *Thermochemical Properties of Inorganic Substances*, Springer-Verlag, Berlin, 1973; J. B. Pedley, R. D. Naylor, and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed., Chapman and Hall, London, 1986; V. Majer and V. Svoboda, *Enthalpies of Vaporization of Organic Compounds*, International Union of Pure and Applied Chemistry, Chemical Data Series No. 32, Blackwell, Oxford, 1985.

### 6.1.1 Some Thermodynamic Relations

**6.1.1.1 Enthalpy of Formation.** Once standard enthalpies are assigned to the elements, it is possible to determine standard enthalpies for compounds. For the reaction:

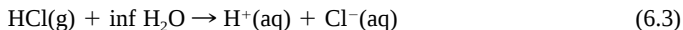


Since the elements are in their standard states, the enthalpy change for the reaction is equal to the standard enthalpy of  $\text{CO}_2$  less the standard enthalpies of C and  $\text{O}_2$ , which are zero in each instance. Thus,

$$\Delta_f H^\circ = -393.51 - 0 - 0 = -393.51 \text{ kJ} \quad (6.2)$$

Tables of enthalpies, such as Tables 6.1 and 6.3, can be used to determine the enthalpy for any reaction at 1 atm and 298.15 K involving the elements and any of the compounds appearing in the tables.

The solution of 1 mole of HCl gas in a large amount of water (infinitely dilute real solution) is represented by:



The heat evolved in the reaction is  $\Delta H^\circ = -74.84 \text{ kJ}$ . With the value of  $\Delta_f H^\circ$  from Table 6.3, one has for the reaction:

$$\Delta_f H^\circ = \Delta_f H^\circ[\text{H}^+(\text{aq})] + \Delta_f H^\circ[\text{Cl}^-(\text{aq})] - \Delta_f H^\circ[\text{HCl}(\text{g})] \quad (6.4)$$

for the standard enthalpy of formation of the pair of ions  $\text{H}^+$  and  $\text{Cl}^-$  in aqueous solution (standard state,  $m = 1$ ). To obtain the  $\Delta_f H^\circ$  values for individual ions, the enthalpy of formation of  $\text{H}^+(\text{aq})$  is arbitrarily assigned the value zero at 298.15 K. Thus, from Eq. (6.4):

$$\Delta_f H^\circ[\text{Cl}^-(\text{aq})] = -74.84 + (-92.31) = -167.15 \text{ kJ}$$

With similar data from Tables 6.1 and 6.3, the enthalpies of formation of other ions can be determined. Thus, from the  $\Delta_f H^\circ[\text{KCl}(\text{aq, std. state, } m = 1 \text{ or aq, ss})]$  of  $-419.53 \text{ kJ}$  and the foregoing value for  $\Delta_f H^\circ[\text{Cl}^-(\text{aq, ss})]$ :

$$\begin{aligned} \Delta_f H^\circ[\text{K}^+(\text{aq, ss})] &= \Delta_f H^\circ[\text{KCl}(\text{aq, ss})] - \Delta_f H^\circ[\text{Cl}^-(\text{aq, ss})] \\ &= -419.53 - (-167.15) = -252.38 \text{ kJ} \end{aligned} \quad (6.5)$$

**6.1.1.2 Enthalpy of Vaporization (or Sublimation)** When the pressure of the vapor in equilibrium with a liquid reaches 1 atm, the liquid boils and is completely converted to vapor on absorption of the enthalpy of vaporization  $\Delta H_v$  at the normal boiling point  $T_b$ . A rough empirical relationship between the normal boiling point and the enthalpy of vaporization (*Trouton's rule*) is:

$$\frac{\Delta H_v}{T_b} = 88 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \quad (6.6)$$

It is best applied to nonpolar liquids which form unassociated vapors.

To a first approximation, the enthalpy of sublimation  $\Delta H_s$  at constant temperature is:

$$\Delta H_s = \Delta H_m + \Delta H_v \quad (6.7)$$

where  $\Delta H_m$  is the enthalpy of melting.

The *Clapeyron* equation expresses the dynamic equilibrium existing between the vapor and the condensed phase of a pure substance:

$$\frac{dP}{dT} = \frac{\Delta H_v}{T\Delta V} \quad (6.8)$$

where  $\Delta V$  is the volume increment between the vapor phase and the condensed phase. If the condensed phase is solid, the enthalpy increment is that of sublimation.

Substitution of  $V = RT/P$  into the foregoing equation and rearranging gives the *Clausius-Clapeyron* equation,

$$\frac{dP}{P dT} = \frac{\Delta H_v}{RT^2} \quad (6.9)$$

or

$$\Delta H_v = -R \frac{d(\ln P)}{1/T} \quad (6.10)$$

which may be used for calculating the enthalpy of vaporization of any compound provided its boiling point at any pressure is known. If an Antoine equation is available (such as Eq. (5.1), page 5.30), differentiation and insertion into the foregoing equation gives:

$$\Delta H_v = \frac{4.5757T^2B}{(T + C - 273.15)^2} \quad (6.11)$$

Inclusion of a compressibility factor into the foregoing equation, as suggested by the *Haggemacher* equation improves the estimate of  $\Delta H_v$ :

$$\Delta H_v = \frac{RT^2}{P} \left( \frac{dP}{dT} \right) \left( 1 - \frac{T_c^3 P}{T^3 P_c} \right)^{1/2} \quad (6.12)$$

where  $T_c$  and  $P_c$  are critical constants (Table 6.5). Although critical constants may be unknown, the compressibility factor is very nearly constant for all compounds belonging to the same family, and an estimate can be deduced from a related compound whose critical constants are available.

**6.1.1.3 Heat Capacity (or Specific Heat)** The temperature dependence of the heat capacity is complex. If the temperature range is restricted, the heat capacity of any phase may be represented adequately by an expression such as:

$$C_p = a + bT + cT^2 \quad (6.13)$$

in which  $a$ ,  $b$ , and  $c$  are empirical constants. These constants may be evaluated by taking three pieces of data:  $(T_1, C_{p,1})$ ,  $(T_2, C_{p,2})$ , and  $(T_3, C_{p,3})$ , and substituting in the following expressions:

$$\frac{C_{p,1}}{(T_1 - T_2)(T_1 - T_3)} + \frac{C_{p,2}}{(T_2 - T_1)(T_2 - T_3)} + \frac{C_{p,3}}{(T_3 - T_2)(T_3 - T_1)} = c \quad (6.14)$$

$$\frac{C_{p,1} - C_{p,2}}{T_1 - T_2} - [(T_1 + T_2)c] = b \quad (6.15)$$

$$(C_{p,1} - bT_1) - cT_1^2 = a \quad (6.16)$$

Smoothed data presented at rounded temperatures, such as are available in Tables 6.2 and 6.4, plus the  $C_p^\circ$  values at 298 K listed in Table 6.1 and 6.3, are especially suitable for substitution in the foregoing parabolic equations. The use of such a parabolic fit is appropriate for interpolation, but data extrapolated outside the original temperature range should not be sought.

**6.1.1.4 Enthalpy of a System** The enthalpy increment of a system over the interval of temperature from  $T_1$  to  $T_2$ , under the constraint of constant pressure, is given by the expression:

$$H_2 - H_1 = \int_{T_1}^{T_2} C_p dT \quad (6.17)$$

The enthalpy over a temperature range that includes phase transitions, melting, and vaporization, is represented by:

$$\begin{aligned} H_2 - H_1 = & \int_{T_1}^{T_2} C_{p(c,II)} dT + \Delta H_t + \int_{T_1}^{T_m} C_{p(c,I)} dT + \Delta H_m \\ & + \int_{T_m}^{T_b} C_{p(1q)} dT + \Delta H_v + \int_{T_b}^{T_2} C_{p(g)} dT \end{aligned} \quad (6.18)$$

Integration of heat capacities, as expressed by Eq. (6.13), leads to:

$$\Delta H = a(T_2 - T_1) + \frac{b(T_2^2 - T_1^2)}{2} + \frac{c(T_2^3 - T_1^3)}{3} \quad (6.19)$$

**6.1.1.5 Entropy** In the physical change of state,

$$\Delta S_m = \frac{\Delta H_m}{T_m} \quad (6.20)$$

is the entropy of melting (or fusion),

$$\Delta S_v = \frac{\Delta H_v}{T_b} \quad (6.21)$$

is the entropy of vaporization, and

$$\Delta S_s = \frac{\Delta H_s}{T_s} \quad (6.22)$$

is the entropy of sublimation.

A general expression for the entropy of a system, involving any phase transitions, is

$$S_2 - S_1 = \int_{T_1}^{T_i} \frac{C_p(c, \text{II})}{T} dT + \frac{\Delta H_t}{T} + \int_{T_b}^{T_m} \frac{C_p(c, \text{I})}{T} dT + \frac{\Delta H_m}{T} \\ + \int_{T_m}^{T_b} \frac{C_p(1q)}{T} dT + \frac{\Delta H_v}{T} + \int_{T_b}^{T_m} \frac{C_p(g)}{T} dT \quad (6.23)$$

If  $C_p$  is independent of temperature,

$$\Delta S = C_p (\ln T_2 - \ln T_1) = 2.303 C_p \log \frac{T_2}{T_1} \quad (6.24)$$

If the heat capacities change with temperature, an empirical equation like Eq. (6.13) may be inserted in Eq. (6.23) before integration. Usually the integration is performed graphically from a plot of either  $C_p/T$  versus  $T$  or  $C_p$  versus  $\ln T$ .

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds

| Substance                    | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Acenaphthene                 | c              | 70.34                                      |                                            | 188.9                                               | 190.4                                                 |
| Acenaphthylene               | c              | 186.7                                      |                                            |                                                     | 166.4                                                 |
| Acetaldehyde                 | lq             | -192.2                                     | -127.6                                     | 160.4                                               | 89.0                                                  |
|                              | g              | -166.1                                     | -133.0                                     | 263.8                                               | 55.3                                                  |
| Acetaldoxime                 | c              | -77.9                                      |                                            |                                                     |                                                       |
|                              | lq             | -81.6                                      |                                            |                                                     |                                                       |
| Acetamide                    | c              | -317.0                                     |                                            | 115.0                                               | 91.3                                                  |
| Acetamidoguanidine nitrate   | c              | -494.0                                     |                                            |                                                     |                                                       |
| 1-Acetamido-2-nitroguanidine | c              | -193.6                                     |                                            |                                                     |                                                       |
| 5-Acetamidotetrazole         | c              | -5.0                                       |                                            |                                                     |                                                       |
| Acetanilide                  | c              | -210.6                                     |                                            |                                                     |                                                       |
| Acetic acid                  | lq             | -484.4                                     | -390.2                                     | 159.9                                               | 123.6                                                 |
|                              | g              | -432.2                                     | -374.2                                     | 283.5                                               | 63.4                                                  |
| ionized; std. state, $m = 1$ | aq             | -486.34                                    | -369.65                                    | 86.7                                                | -6.3                                                  |
| Acetic anhydride             | lq             | -624.4                                     | -489.14                                    | 268.8                                               | 168.2 <sup>30</sup>                                   |
| Acetone                      | lq             | -248.4                                     | -152.7                                     | 198.8                                               | 126.3                                                 |
|                              | g              | -217.1                                     | -152.7                                     | 295.3                                               | 74.5                                                  |
| Acetonitrile                 | lq             | 31.4                                       | 86.5                                       | 149.7                                               | 91.5                                                  |
|                              | g              | 74.0                                       | 91.9                                       | 243.4                                               | 52.2                                                  |
| Acetophenone                 | lq             | -142.5                                     | -17.0                                      | 249.6                                               | 204.6                                                 |
| Acetyl bromide               | lq             | -223.5                                     |                                            |                                                     |                                                       |
| Acetyl chloride              | lq             | -272.9                                     | -208.2                                     | 201.0                                               | 117.0                                                 |
|                              | g              | -242.8                                     | -205.8                                     | 295.1                                               | 67.8                                                  |
| Acetylene                    | g              | 227.4                                      | 209.0                                      | 201.0                                               | 44.1                                                  |
| Acetylene- $d_2$             | g              | 221.5                                      | 205.9                                      | 208.9                                               | 49.3                                                  |
| Acetylenedicarboxylic acid   | c              | -578.2                                     |                                            |                                                     |                                                       |
| Acetyl fluoride              | g              | -442.1                                     |                                            |                                                     |                                                       |
| 1-Acetylimidazole            | c              | -574.0                                     |                                            |                                                     |                                                       |
| Acetyl iodide                | lq             | -163.5                                     |                                            |                                                     |                                                       |
| Acridine                     | c              | 179.4                                      |                                            |                                                     |                                                       |
| Adamantane                   | c              | -194.1                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                     | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Adenine                                       | c              | 96.0                                       | 299.6                                      | 151.1                                               | 147.0                                                 |
| (+)-Alanine                                   | c              | -561.2                                     | -369.4                                     | 132.3                                               |                                                       |
| (-)-Alanine                                   | c              | -604.0                                     | -370.5                                     | 129.3                                               |                                                       |
| (±)-Alanine                                   | c              | -563.6                                     | -372.3                                     | 132.3                                               |                                                       |
| β-Alanine                                     | c              | -558.0                                     |                                            |                                                     |                                                       |
| (±)-N-Alanylglycine                           | c              | -777.8                                     | -489.9                                     | 213.5                                               |                                                       |
| (-)-Alanylglycine                             | c              | -827.0                                     | -533.0                                     | 195.2                                               |                                                       |
| Allene                                        | g              | 190.5                                      |                                            |                                                     |                                                       |
| Alloxan monohydrate                           | c              | -1000.7                                    | -762.3                                     | 186.7                                               |                                                       |
| Allylamine                                    | lq             | -10.0                                      |                                            |                                                     |                                                       |
| Allyl <i>tert</i> -butyl sulfide              | lq             | -91.0                                      |                                            |                                                     |                                                       |
| Allyl ethyl sulfone                           | lq             | -406.0                                     |                                            |                                                     |                                                       |
| Allyl methyl sulfone                          | lq             | -385.1                                     |                                            |                                                     |                                                       |
| Allyl trichloroacetate                        | lq             | -395.3                                     |                                            |                                                     |                                                       |
| Allyl ( <i>see</i> Propene)                   |                |                                            |                                            |                                                     |                                                       |
| Aminetrimethylboron                           | c              | -284.1                                     | -79.3                                      | 218.0                                               |                                                       |
| 3-Aminoacetophenone                           | c              | -173.3                                     |                                            |                                                     |                                                       |
| 4-Aminoacetophenone                           | c              | -182.1                                     |                                            |                                                     |                                                       |
| 2-Aminoacridine                               | c              | 166.4                                      |                                            |                                                     |                                                       |
| 9-Aminoacridine                               | c              | 159.2                                      |                                            |                                                     |                                                       |
| 2-Aminobenzoic acid                           | c              | -400.9                                     |                                            |                                                     |                                                       |
| 3-Aminobenzoic acid                           | c              | -411.6                                     |                                            |                                                     |                                                       |
| 4-Aminobenzoic acid                           | c              | -412.9                                     |                                            |                                                     |                                                       |
| 2-Aminobiphenyl                               | c              | 112.2                                      |                                            |                                                     |                                                       |
| 4-Aminobiphenyl                               | c              | 81.2                                       |                                            |                                                     |                                                       |
| 4-Aminobutanoic acid                          | c              | -581.0                                     |                                            |                                                     |                                                       |
| 2-Aminoethanesulfonic acid                    | c              | -785.9                                     | -562.3                                     | 154.1                                               | 140.7                                                 |
| ionized; std. state, <i>m</i> = 1             | aq             | -719.8                                     | -509.8                                     | 200.1                                               |                                                       |
| 2-Aminoethanol                                | lq             |                                            |                                            |                                                     | 195.5                                                 |
| 2-Aminohexanoic acid<br>(norleucine)          | c              | -639.1                                     |                                            |                                                     |                                                       |
| 4-Aminohexanoic acid                          | c              | -646.2                                     |                                            |                                                     |                                                       |
| 5-Aminohexanoic acid                          | c              | -643.3                                     |                                            |                                                     |                                                       |
| 6-Aminohexanoic acid                          | c              | -639.1                                     |                                            |                                                     |                                                       |
| (-)-2-Amino-3-hydroxy-<br>butanoic acid       | c              | -759.5                                     |                                            |                                                     |                                                       |
| 2-Amino-2-(hydroxymethyl)-<br>1,1-propanediol | c              | 717.8                                      |                                            |                                                     |                                                       |
| 3-Aminonitroguanidine                         | c              | 22.1                                       |                                            |                                                     |                                                       |
| 5-Aminopentanoic acid                         | c              | -604.1                                     |                                            |                                                     |                                                       |
| 5-Aminotetrazole                              | c              | -207.8                                     |                                            |                                                     |                                                       |
| 3-Amino-1,2,4-triazole                        | c              | 76.8                                       |                                            |                                                     |                                                       |
| Aniline                                       | lq             | 31.3                                       | 149.2                                      | 191.4                                               | 191.9                                                 |
|                                               | g              | 87.5                                       | -7.0                                       | 317.9                                               | 107.9                                                 |
| Anthracene                                    | c              | 129.2                                      | 286.0                                      | 207.6                                               | 210.5                                                 |
| 9,10-Anthraquinone                            | c              | -207.5                                     |                                            |                                                     |                                                       |
| D(-)-Arabinose [also (+)-]                    | c              | -1057.9                                    |                                            |                                                     |                                                       |
| (+)-Arginine                                  | c              | -623.5                                     | -240.5                                     | 250.8                                               | 232.0                                                 |
| L-(+)-Ascorbic acid                           | c              | -1164.6                                    |                                            |                                                     |                                                       |
| L-(+)-Asparagine                              | c              | -789.4                                     | -530.6                                     | 174.6                                               |                                                       |
| L-(+)-Aspartic acid                           | c              | -973.3                                     | -730.7                                     | 170.2                                               |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                            | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| <i>cis</i> -Azobenzene               | c              | 310.2                                      |                                            |                                                     |                                                       |
| <i>trans</i> -Azobenzene             | c              | 365.2                                      |                                            |                                                     |                                                       |
| Azoisopropane                        | g              | 35.8                                       |                                            |                                                     |                                                       |
| Azomethane                           | g              | 148.8                                      | 239.7                                      | 289.9                                               | 78.0                                                  |
| Azomethane- <i>d</i> <sub>6</sub>    | g              | 119.3                                      | 218.3                                      | 305.7                                               | 90.6                                                  |
| Azopropane                           | g              | 51.5                                       |                                            |                                                     |                                                       |
| Azulene                              | c              | 289.1                                      | 353.4                                      | 338.1                                               | 128.5                                                 |
| Barbituric acid                      | c              | -637.2                                     |                                            |                                                     |                                                       |
| Benzaldehyde                         | lq             | -87.0                                      | 9.4                                        |                                                     | 172.0                                                 |
| Benzamide                            | c              | -202.6                                     |                                            |                                                     |                                                       |
| Benzanilide                          | c              | -93.4                                      |                                            |                                                     |                                                       |
| 1,2-Benzanthracene                   | c              | 170.9                                      |                                            |                                                     |                                                       |
| 2,3-Benzanthracene                   | c              | 160.4                                      | 359.2                                      | 215.5                                               |                                                       |
| 1,2-Benzanthracene-9,10-dione        | c              | -231.9                                     |                                            |                                                     |                                                       |
| Benzene                              | lq             | 49.0                                       | 124.4                                      | 173.4                                               | 136.0                                                 |
|                                      | g              | 82.6                                       | 129.7                                      | 269.2                                               | 82.4                                                  |
| Benzeneboronic acid                  | c              | -720.1                                     |                                            |                                                     |                                                       |
| 1,2-Benzenediamine                   | c              | -0.3                                       |                                            |                                                     |                                                       |
| 1,3-Benzenediamine                   | c              | -7.8                                       |                                            |                                                     |                                                       |
| 1,4-Benzenediamine                   | c              | 3.1                                        |                                            |                                                     |                                                       |
| 1,3-Benzenedicarboxylic acid         | c              | 803.0                                      |                                            |                                                     |                                                       |
| 1,4-Benzenedicarboxylic acid         | c              | 816.1                                      |                                            |                                                     |                                                       |
| 1,2,4,5-Benzenetetra-carboxylic acid | c              | 1571.0                                     |                                            |                                                     |                                                       |
| Benzenethiol (thiophenol)            | lq             | 63.7                                       | 134.0                                      | 222.8                                               | 173.2                                                 |
|                                      | g              | 111.3                                      | 147.6                                      | 336.9                                               | 104.9                                                 |
| 1,2,3-Benzenetricarboxylic acid      | c              | -1160.0                                    |                                            |                                                     |                                                       |
| 1,2,4-Benzenetricarboxylic acid      | c              | -1179.0                                    |                                            |                                                     |                                                       |
| 1,3,5-Benzenetricarboxylic acid      | c              | -1190.0                                    |                                            |                                                     |                                                       |
| 1,2,3-Benzenetriol                   | c              | -551.1                                     |                                            |                                                     |                                                       |
| 1,2,4-Benzenetriol                   | c              | -563.8                                     |                                            |                                                     |                                                       |
| 1,3,5-Benzenetriol                   | c              | -584.6                                     |                                            |                                                     |                                                       |
| <i>p</i> -Benzidine                  | c              | 70.7                                       |                                            |                                                     |                                                       |
| Benzil                               | c              | -153.9                                     |                                            |                                                     |                                                       |
| Benzoic acid                         | c              | -385.2                                     | -245.3                                     | 167.6                                               | 146.8                                                 |
| Benzoic anhydride                    | c              | -415.4                                     |                                            |                                                     |                                                       |
| Benzonitrile                         | lq             | 163.2                                      |                                            | 209.1                                               | 165.2                                                 |
|                                      | g              | 215.8                                      | 260.8                                      | 321.0                                               | 109.1                                                 |
| Benzo[ <i>def</i> ]phenanthrene      | c              | 125.5                                      | 269.5                                      | 224.8                                               | 236.0                                                 |
| Benzophenone                         | c              | -34.5                                      | 140.2                                      | 245.2                                               | 224.8                                                 |
| Benzo[ <i>f</i> ]quinoline           | c              | 150.6                                      |                                            |                                                     |                                                       |
| Benzo[ <i>h</i> ]quinoline           | c              | 149.7                                      |                                            |                                                     |                                                       |
| 1,4-Benzoquinone                     | c              | -185.7                                     | -83.6                                      | 162.8                                               | 129.0                                                 |
| Benzo[ <i>b</i> ]thiophene           | c              | 100.6                                      |                                            |                                                     |                                                       |
| 1,2,3-Benzotriazole                  | c              | 250.0                                      |                                            |                                                     |                                                       |
| Benzotrifluoride                     | lq             | -636.7                                     |                                            |                                                     |                                                       |
| Benzoyl bromide                      | lq             | -107.3                                     |                                            |                                                     |                                                       |
| Benzoyl chloride                     | lq             | -158.0                                     |                                            |                                                     |                                                       |
| Benzoylformic acid                   | c              | -482.4                                     |                                            |                                                     |                                                       |
| <i>N</i> -Benzoylglycine             | c              | -609.8                                     | -369.57                                    | 239.3                                               |                                                       |



**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                              | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Benzoyl iodide                         | lq             | − 53.5                                     |                                            |                                                     |                                                       |
| 3,4-Benzphenanthrene                   | c              | 184.9                                      |                                            |                                                     |                                                       |
| Benzylamine                            | lq             | 34.2                                       |                                            |                                                     |                                                       |
| Benzyl alcohol                         | lq             | − 160.7                                    | − 27.5                                     | 216.7                                               | 218.0                                                 |
| Benzyl bromide                         | lq             | 16.0                                       |                                            |                                                     |                                                       |
| Benzyl chloride                        | lq             | − 32.6                                     |                                            |                                                     | 182.4                                                 |
| N-Benzyl diphenylamine                 | c              | 184.7                                      |                                            |                                                     |                                                       |
| Benzyl ethyl sulfide                   | lq             | − 4.9                                      |                                            |                                                     |                                                       |
| Benzyl iodide                          | lq             | 57.3                                       |                                            |                                                     |                                                       |
| Benzyl methyl ketone                   | lq             | − 151.9                                    |                                            |                                                     |                                                       |
| Benzyl methyl sulfide                  | lq             | 26.2                                       |                                            |                                                     |                                                       |
| Bicyclo[1.1.0]butane                   | g              | 217.1                                      |                                            |                                                     |                                                       |
| Bicyclo[2.2.1]hepta-2,5-dione          | lq             | 213.0                                      |                                            |                                                     |                                                       |
| Bicyclo[2.2.1]heptane                  | c              | − 95.1                                     |                                            |                                                     |                                                       |
| Bicyclo[4.1.0]heptane                  | lq             | − 36.7                                     |                                            |                                                     |                                                       |
| Bicyclo[2.2.1]heptene                  | lq             | 90.0                                       | 203.9                                      |                                                     | 130.0                                                 |
| Bicyclo[3.1.0]hexane                   | g              | 38.6                                       |                                            |                                                     |                                                       |
| Bicyclohexyl                           | lq             | − 273.7                                    |                                            |                                                     |                                                       |
| Bicyclo[2.2.2]octane                   | c              | − 146.9                                    |                                            |                                                     |                                                       |
| Bicyclo[4.2.0]octane                   | g              | − 26.2                                     |                                            |                                                     |                                                       |
| Bicyclo[5.1.0]octane                   | g              | − 16.6                                     |                                            |                                                     |                                                       |
| Bicyclo[2.2.2]oct-2-ene                | g              | − 23.3                                     |                                            |                                                     |                                                       |
| Bicyclopropyl                          | g              | 129.3                                      |                                            |                                                     |                                                       |
| Biphenyl                               | c              | 99.4                                       | 254.2                                      | 209.4                                               | 198.4                                                 |
| 2-Biphenylcarboxylic acid              | c              | − 349.0                                    |                                            |                                                     |                                                       |
| (1,1'-Biphenyl)-4,4'-diamine           | c              | 70.7                                       |                                            |                                                     |                                                       |
| Biphenylene                            | c              | 334.0                                      |                                            |                                                     |                                                       |
| Bis(2-chloroethyl) ether               | lq             |                                            |                                            |                                                     | 220.9                                                 |
| Bis(dimethylthiocarbonyl) disulfide    | c              | 41.6                                       |                                            |                                                     |                                                       |
| Bis(2-hydroxyethyl) ether              | lq             | − 1621.0                                   |                                            | 441.0                                               | 135.1                                                 |
|                                        | g              | − 571.1                                    |                                            |                                                     |                                                       |
| Bromoacetone                           | g              | − 181.0                                    |                                            |                                                     |                                                       |
| Bromoacetylene                         | g              |                                            |                                            | 253.7                                               | 55.7                                                  |
| Bromobenzene                           | lq             | 60.9                                       | 126.0                                      | 219.2                                               | 154.3                                                 |
| 4-Bromobenzoic acid                    | c              | − 378.3                                    |                                            |                                                     |                                                       |
| 1-Bromobutane                          | lq             | − 143.8                                    | − 12.9                                     | 369.8                                               | 109.3                                                 |
| 2-Bromobutane                          | lq             | − 154.8                                    | − 19.25                                    |                                                     |                                                       |
|                                        | g              | − 120.3                                    | − 25.8                                     | 370.3                                               | 110.8                                                 |
| Bromochlorodifluoromethane             | g              | − 471.5                                    | − 448.4                                    | 318.5                                               | 74.6                                                  |
| 1-Bromo-2-chloroethane                 | lq             |                                            |                                            |                                                     | 130.1 <sup>27</sup>                                   |
| Bromochlorofluoromethane               | g              | − 295.0                                    | − 278.6                                    | 304.3                                               | 63.2                                                  |
| Bromochloromethane                     | lq             |                                            |                                            |                                                     | 52.7                                                  |
|                                        | g              | − 50.2                                     | − 39.3                                     | 287.6                                               |                                                       |
| 1-Bromo-2-chloro-1,1,2-trifluoroethane | g              | − 644.8                                    |                                            |                                                     |                                                       |
| 2-Bromo-2-chloro-1,1,1-trifluoroethane | g              | − 690.4                                    |                                            |                                                     |                                                       |
| 1-Bromodecane                          | lq             | − 344.7                                    |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                     | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Bromodichlorofluoromethane    | g              | -269.5                                     | -246.8                                     | 330.6                                               | 80.0                                                  |
| Bromodichloromethane          | g              | -58.6                                      | -42.5                                      | 316.4                                               | 67.4                                                  |
| Bromodifluoromethane          | g              | -424.9                                     | -447.3                                     | 295.1                                               | 58.7                                                  |
| Bromoethane                   | lq             | -90.5                                      | -25.8                                      | 198.7                                               | 100.8                                                 |
|                               | g              | -61.9                                      | -23.9                                      | 286.7                                               | 64.5                                                  |
| Bromoethylene (vinyl bromide) | lq             |                                            |                                            |                                                     | 107.7 <sup>15</sup>                                   |
|                               | g              | 79.2                                       | 81.7                                       | 275.8                                               | 55.4                                                  |
| Bromofluoromethane            | g              | -252.7                                     | -241.5                                     | 276.3                                               | 49.2                                                  |
| 1-Bromoheptane                | lq             | -218.4                                     |                                            |                                                     |                                                       |
| 1-Bromohexane                 | lq             | -194.2                                     |                                            | 453.0                                               | 203.5                                                 |
| Bromiodomethane               | g              | 50.2                                       | 39.2                                       | 307.5                                               |                                                       |
| Bromomethane                  | lq             |                                            |                                            |                                                     | 78.7 <sup>7</sup>                                     |
|                               | g              | -35.4                                      | -26.3                                      | 246.4                                               | 42.5                                                  |
| 2-Bromo-2-methylpropane       | lq             | -163.8                                     |                                            |                                                     | 151.0                                                 |
|                               | g              | -132.4                                     | -28.2                                      | 332.0                                               | 116.5                                                 |
| 1-Bromooctane                 | lq             | -245.1                                     |                                            |                                                     |                                                       |
| Bromopentafluoroethane        | g              | -1064.4                                    |                                            |                                                     |                                                       |
| 1-Bromopentane                | lq             | -170.2                                     |                                            |                                                     | 132.2                                                 |
|                               | g              | -129.0                                     | -5.7                                       | 408.8                                               |                                                       |
| 1-Bromopropane                | lq             | -121.8                                     |                                            |                                                     | 86.4                                                  |
|                               | g              | -87.0                                      | -22.5                                      | 330.9                                               |                                                       |
| 2-Bromopropane                | lq             | -130.5                                     |                                            |                                                     | 132.2                                                 |
|                               | g              | -99.4                                      | -27.2                                      | 316.2                                               | 89.4                                                  |
| cis-1-Bromopropene            | g              | 40.8                                       |                                            |                                                     |                                                       |
| 3-Bromopropene                | g              | 45.2                                       |                                            |                                                     |                                                       |
| N-Bromosuccinimide            | c              | -335.9                                     |                                            |                                                     |                                                       |
| $\alpha$ -Bromotoluene        | lq             | 23.4                                       |                                            |                                                     |                                                       |
| Bromotrichloromethane         | g              | -41.1                                      | -12.4                                      | 332.8                                               | 85.3                                                  |
| Bromotrifluoroethane          | g              | -694.5                                     |                                            |                                                     |                                                       |
| Bromotrifluoromethane         | g              | -648.3                                     | -622.6                                     | 297.8(5)                                            | 69.3                                                  |
| Bromotrimethylsilane          | lq             | -325.9                                     |                                            |                                                     |                                                       |
| Bromotrinitromethane          | g              | 80.3                                       |                                            |                                                     |                                                       |
| Brucine                       | c              | -496.2                                     |                                            |                                                     |                                                       |
| 1,2-Butadiene                 | g              | 162.3                                      | 199.5                                      | 293.0                                               | 80.1                                                  |
| 1,3-Butadiene                 | lq             | 88.5                                       |                                            | 199.0                                               | 123.6                                                 |
|                               | g              | 110.0                                      | 150.7                                      | 278.7                                               | 79.5                                                  |
| 1,3-Butadiyne                 | g              | 472.8                                      | 444.0                                      | 250.0                                               | 73.6                                                  |
| Butanal                       | lq             | -239.2                                     |                                            |                                                     | 163.7                                                 |
|                               | g              | -204.9                                     | -114.8                                     | 243.7                                               | 103.4                                                 |
| Butanamide                    | lq             | -346.9                                     |                                            |                                                     |                                                       |
| Butane                        | lq             |                                            |                                            |                                                     | 104.5 <sup>-0.5</sup>                                 |
|                               | g              | -125.6                                     | -17.2                                      | 310.1                                               | 97.5                                                  |
| 1,2-Butanediamine             | lq             | -120.2                                     |                                            |                                                     |                                                       |
| ( $\pm$ )-1,2-Butanediol      | lq             | -523.6                                     |                                            |                                                     |                                                       |
| 1,3-Butanediol                | lq             | -501.0                                     |                                            |                                                     | 227.2 <sup>30</sup>                                   |
| 1,4-Butanediol                | lq             | -503.3                                     |                                            | 223.4                                               | 200.1                                                 |
| 2,3-Butanediol                | lq             | -541.5                                     |                                            |                                                     | 213.0                                                 |
| Butanedinitrile               | c              | 139.7                                      |                                            |                                                     |                                                       |
|                               | lq             |                                            |                                            |                                                     | 160.5 <sup>62</sup>                                   |
| 2,3-Butanedione               | lq             | -365.8                                     |                                            |                                                     |                                                       |
| 1,4-Butanedithiol             | lq             | -105.7                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Butanenitrile            | lq             | − 5.8                                      |                                            |                                                     | 159 <sup>67</sup>                                     |
|                          | g              | 33.6                                       | 108.7                                      | 325.4                                               | 97.0                                                  |
| 1-Butanethiol            | lq             | − 124.7                                    | 4.1                                        | 276.0                                               | 171.2                                                 |
| 2-Butanethiol            | lq             | − 131.0                                    | − 0.17                                     | 271.4                                               |                                                       |
| Butanoic acid            | lq             | − 533.8                                    | − 377.7                                    | 222.2                                               | 178.6                                                 |
| Butanoic anhydride       | lq             |                                            |                                            |                                                     | 283.7                                                 |
| 1-Butanol                | lq             | − 327.3                                    | − 162.5                                    | 225.8                                               | 177.0                                                 |
|                          | g              | − 275.0                                    | − 150.8                                    | 362.8                                               | 122.6                                                 |
| (±)-2-Butanol            | lq             | − 342.6                                    | − 177.0                                    | 214.9                                               | 196.9                                                 |
|                          | g              | − 292.9                                    | − 167.6                                    | 359.5                                               | 113.3                                                 |
| 2-Butanone               | lq             | − 273.3                                    | − 151.4                                    | 239.1                                               | 158.9                                                 |
|                          | g              | − 238.5                                    |                                            | 339.9                                               | 101.7                                                 |
| Butanophenone            | lq             | − 188.9                                    |                                            |                                                     |                                                       |
| trans-2-Butenal          | lq             | − 138.7                                    |                                            |                                                     | 95.4                                                  |
| cis-Butenedinitrile      | c              | 268.2                                      |                                            |                                                     |                                                       |
| 1-Butene                 | lq             | − 20.8                                     |                                            | 227.0                                               | 118.0                                                 |
|                          | g              | 0.1                                        | 71.3                                       | 305.6                                               | 85.7                                                  |
| cis-2-Butene             | lq             | − 29.8                                     |                                            | 219.9                                               | 127.0                                                 |
|                          | g              | − 7.1                                      | 65.9                                       | 300.8                                               | 78.9                                                  |
| trans-2-Butene           | g              | − 11.4                                     | 63.0                                       | 296.5                                               | 87.8                                                  |
| cis-2-Butenenitrile      | lq             | 95.1                                       |                                            |                                                     |                                                       |
| trans-2-Butenenitrile    | lq             | 95.1                                       |                                            |                                                     |                                                       |
| 3-Butenenitrile          | g              | 159.7                                      | 193.4                                      | 298.4                                               | 82.1                                                  |
| cis-2-Butenoic acid      | lq             | − 347.0                                    |                                            |                                                     |                                                       |
| trans-2-Butenoic acid    | c              | − 430.5                                    |                                            |                                                     |                                                       |
| cis-2-Butenedioic acid   | c              | − 788.7                                    |                                            |                                                     |                                                       |
| trans-2-Butenedioic acid | c              | − 811.1                                    |                                            |                                                     |                                                       |
| 1-Buten-3-yne            | g              | 304.6                                      | 306.0                                      | 279.4                                               | 73.2                                                  |
| 2-Butoxyethanol          | lq             |                                            |                                            |                                                     | 281.0                                                 |
| N-Butylacetamide         | lq             | − 380.8                                    |                                            |                                                     |                                                       |
| Butyl acetate            | lq             | − 529.2                                    |                                            |                                                     | 227.8                                                 |
| Butylamine               | lq             | − 127.7                                    |                                            |                                                     | 179.2                                                 |
|                          | g              | − 92.0                                     | 49.2                                       | 363.3                                               | 118.6                                                 |
| sec-Butylamine           | lq             | − 137.5                                    |                                            |                                                     |                                                       |
|                          | g              | − 104.6                                    | 40.7                                       | 351.3                                               | 117.2                                                 |
| tert-Butylamine          | g              | − 150.6                                    |                                            |                                                     | 192.1                                                 |
|                          | g              | − 121.0                                    | 28.9                                       | 337.9                                               | 120.0                                                 |
| Butylbenzene             | lq             | 63.2                                       |                                            |                                                     | 243.4                                                 |
|                          | g              | − 13.1                                     | 144.7                                      | 439.5                                               | 416.3                                                 |
| sec-Butylbenzene         | lq             | − 66.4                                     |                                            |                                                     |                                                       |
| tert-Butylbenzene        | lq             | − 70.7                                     |                                            |                                                     | 238.0                                                 |
| sec-Butyl butanoate      | lq             | − 492.6                                    |                                            |                                                     |                                                       |
| Butyl chloroacetate      | lq             | − 538.4                                    |                                            |                                                     |                                                       |
| Butyl 2-chlorobutanoate  | lq             | − 655.2                                    |                                            |                                                     |                                                       |
| Butyl 3-chlorobutanoate  | lq             | − 610.9                                    |                                            |                                                     |                                                       |
| Butyl 4-chlorobutanoate  | lq             | − 618.0                                    |                                            |                                                     |                                                       |
| Butyl 2-chloropropanoate | lq             | − 572.0                                    |                                            |                                                     |                                                       |
| Butyl 3-chloropropanoate | lq             | − 558.2                                    |                                            |                                                     |                                                       |
| Butyl crotonate          | lq             | − 467.8                                    |                                            |                                                     |                                                       |
| Butylcyclohexane         | lq             | − 263.1                                    |                                            | 345.0                                               | 271.0                                                 |
|                          | g              | − 213.4                                    | 56.4                                       | 458.5                                               | 207.1                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                         | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Butylcyclopentane                 | g              | -168.3                                     | 61.4                                       | 456.2                                               | 177.5                                                 |
| Butyl dichloroacetate             | lq             | -550.2                                     |                                            |                                                     |                                                       |
| Butyl ethyl ether                 | lq             |                                            |                                            |                                                     | 159.0                                                 |
| Butyl ethyl sulfide               | g              | -125.2                                     | 32.0                                       | 453.0                                               | 162.0                                                 |
| (3-thiaheptane)                   |                |                                            |                                            |                                                     |                                                       |
| <i>tert</i> -Butyl ethyl sulfide  | lq             | -187.3                                     |                                            |                                                     |                                                       |
| Butyl formate                     | lq             |                                            |                                            |                                                     | 200.2                                                 |
| <i>tert</i> -Butyl hydroperoxide  | lq             | -293.6                                     |                                            |                                                     |                                                       |
| Butyllithium                      | lq             | -132.2                                     |                                            |                                                     |                                                       |
| Butyl methyl ether                | lq             | -290.6                                     |                                            | 295.3                                               | 192.7                                                 |
| <i>tert</i> -Butyl methyl ether   | lq             | -313.6                                     |                                            | 265.3                                               | 187.5                                                 |
| Butyl methyl sulfide              | lq             | -142.8                                     | 17.1                                       | 307.5                                               | 200.9                                                 |
| (2-thiahexane)                    |                |                                            |                                            |                                                     |                                                       |
| <i>tert</i> -Butyl methyl sulfide | lq             | -156.9                                     |                                            | 276.1                                               | 199.9                                                 |
| Butyl methyl sulfone              | lq             | -535.8                                     |                                            |                                                     |                                                       |
| <i>tert</i> -Butyl methyl sulfone | c              | -556.0                                     |                                            |                                                     |                                                       |
| <i>cis</i> -Butyl 9-octadecanoate | lq             | -816.9                                     |                                            |                                                     |                                                       |
| <i>tert</i> -Butyl peroxide       | lq             | -380.9                                     |                                            |                                                     |                                                       |
| Butyl trichloroacetate            | lq             | -545.8                                     |                                            |                                                     |                                                       |
| Butylurea                         | c              | -419.5                                     |                                            |                                                     |                                                       |
| Butyl vinyl ether                 | lq             | -218.8                                     |                                            |                                                     | 232.0                                                 |
| 1-Butyne                          | g              | 165.2                                      | 202.1                                      | 290.8                                               | 81.4                                                  |
| 2-Butyne                          | g              | 145.7                                      | 185.4                                      | 283.3                                               | 78.0                                                  |
| 2-Butynedinitrile                 | g              | 529.2                                      |                                            |                                                     |                                                       |
| 2-Butynedioic acid                | c              | -577.4                                     |                                            |                                                     |                                                       |
| 3-Butynoic acid                   | c              | -241.8                                     |                                            |                                                     |                                                       |
| $\gamma$ -Butyrolactone           | lq             | -420.9                                     |                                            |                                                     | 141.4                                                 |
| (+)-Camphor                       | c              | -319.4                                     |                                            |                                                     | 271.2                                                 |
| $\epsilon$ -Caprolactam           | c              | -329.4                                     |                                            |                                                     |                                                       |
| 9 <i>H</i> -Carbazole             | c              | 101.7                                      |                                            |                                                     |                                                       |
| Carbonyl bromide                  | g              | -96.2                                      | -110.9                                     | 309.1                                               | 61.8                                                  |
| Carbonyl chloride                 | g              | -219.1                                     | -204.9                                     | 283.5                                               | 57.7                                                  |
| Carbonyl chloride fluoride        | g              |                                            |                                            | 276.7                                               | 52.4                                                  |
| Carbonyl fluoride                 | g              | -639.8                                     |                                            |                                                     | 46.8                                                  |
| Chloroacetamide                   | c              | -338.5                                     |                                            |                                                     |                                                       |
| Chloroacetic acid                 | c              | -510.5                                     |                                            |                                                     |                                                       |
| Chloroacetyl chloride             | lq             | -283.7                                     |                                            |                                                     |                                                       |
| Chloroacetylene                   | g              |                                            |                                            | 242.0                                               | 54.3                                                  |
| 2-Chlorobenzaldehyde              | lq             | -118.4                                     |                                            |                                                     |                                                       |
| 3-Chlorobenzaldehyde              | lq             | -126.0                                     |                                            |                                                     |                                                       |
| 4-Chlorobenzaldehyde              | c              | -146.4                                     |                                            |                                                     |                                                       |
| Chlorobenzene                     | lq             | 11.0                                       | 89.2                                       | 209.2                                               | 150.2                                                 |
| 2-Chlorobenzoic acid              | c              | -404.5                                     |                                            |                                                     |                                                       |
| 3-Chlorobenzoic acid              | c              | -423.3                                     |                                            |                                                     |                                                       |
| 4-Chlorobenzoic acid              | c              | -428.9                                     |                                            |                                                     | 163.2                                                 |
| Chloro-1,4-benzoquinone           | c              | -220.6                                     |                                            |                                                     |                                                       |
| 1-Chlorobutane                    | lq             | -188.1                                     |                                            |                                                     | 175.0                                                 |
|                                   | g              | -154.6                                     | -38.8                                      | 358.1                                               | 107.6                                                 |
| ( $\pm$ )-2-Chlorobutane          | lq             | -192.8                                     |                                            |                                                     |                                                       |
|                                   | g              | -161.2                                     | -53.5                                      | 359.6                                               | 108.5                                                 |
| 2-Chlorobutanoic acid             | lq             | -575.5                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                       | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|---------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 3-Chlorobutanoic acid           | lq             | − 556.3                                    |                                            |                                                     |                                                       |
| 4-Chlorobutanoic acid           | lq             | − 566.3                                    |                                            |                                                     |                                                       |
| Chlorocyclohexane               | lq             | − 207.2                                    |                                            |                                                     |                                                       |
| 1-Chloro-1,1-difluoroethane     | lq             |                                            |                                            |                                                     | 130.5 <sup>21</sup>                                   |
|                                 | g              |                                            |                                            | 307.2                                               | 82.5                                                  |
| 1-Chloro-2,2-difluoroethylene   | g              | − 315.5                                    | − 289.1                                    | 303.0                                               | 72.1                                                  |
| 2-Chloro-1,1-difluoroethylene   | g              | − 331.4                                    | − 305.0                                    | 302.4                                               |                                                       |
| Chlorodifluoromethane           | lq             |                                            |                                            |                                                     | 93.0 <sup>-41</sup>                                   |
|                                 | g              | − 482.6                                    | − 450.0                                    | 281.0                                               | 55.9                                                  |
| 2-Chloro-1,4-dihydroxybenzene   | c              | − 382.81                                   |                                            |                                                     |                                                       |
| Chlorodimethylsilane            | lq             | − 79.8                                     |                                            |                                                     |                                                       |
| 1-Chloro-2,3-epoxypropane       | lq             | − 148.5                                    |                                            |                                                     | 125.1                                                 |
| 1-Chloroethane                  | lq             | − 136.8                                    | − 59.3                                     | 190.8                                               | 104.3                                                 |
|                                 | g              | − 112.1                                    | − 60.5                                     | 275.8                                               | 62.6                                                  |
| 2-Chloroethanol                 | lq             | − 295.4                                    |                                            |                                                     |                                                       |
| 1-Chloro-2-ethylbenzene         | lq             | − 54.1                                     |                                            |                                                     |                                                       |
| 1-Chloro-4-ethylbenzene         | lq             | − 51.7                                     |                                            |                                                     |                                                       |
| Chloroethylene (vinyl chloride) | lq             |                                            |                                            |                                                     | 89.4                                                  |
|                                 | g              | 37.3                                       | 53.6                                       | 263.9                                               | 53.7                                                  |
| 2-Chloroethyl ethyl ether       | g              | − 301.3                                    |                                            |                                                     |                                                       |
| 2-Chloroethyl vinyl ether       | g              | − 170.1                                    |                                            |                                                     |                                                       |
| Chloroethyne                    | g              | 213.0                                      | 197.0                                      | 241.9                                               | 54.3                                                  |
| 1-Chloro-1-fluoroethane         | g              | − 313.4                                    |                                            |                                                     |                                                       |
| 2-Chlorohexane                  | lq             | − 246.1                                    |                                            |                                                     |                                                       |
| Chlorofluoromethane             | g              | − 290.8                                    | − 265.5                                    | 264.3                                               | 47.0                                                  |
| Chlorohydroquinone              | c              | − 382.8                                    |                                            |                                                     |                                                       |
| Chloriodomethane                | g              | 12.6                                       | 15.4                                       | 296.1                                               |                                                       |
| Chloromethane                   | lq             |                                            |                                            |                                                     | 75.6 <sup>-24</sup>                                   |
|                                 | g              | − 81.9                                     | − 58.5                                     | 234.6                                               | 40.8                                                  |
| 1-Chloro-3-methylbutane         | lq             | − 216.0                                    |                                            |                                                     | 175.1                                                 |
|                                 | g              | − 179.7                                    |                                            |                                                     |                                                       |
| 2-Chloro-2-methylbutane         | g              | − 202.2                                    |                                            |                                                     |                                                       |
| 2-Chloro-3-methylbutane         | g              | − 185.1                                    |                                            |                                                     |                                                       |
| 1-Chloro-2-methylpropane        | lq             | − 191.1                                    |                                            |                                                     | 158.6                                                 |
|                                 | g              | − 159.4                                    | − 49.7                                     | 355.0                                               | 108.5                                                 |
| 2-Chloro-2-methylpropane        | lq             | − 211.2                                    |                                            |                                                     | 172.8                                                 |
|                                 | g              | − 182.2                                    | − 64.1                                     | 322.2                                               | 114.2                                                 |
| 1-Chloronaphthalene             | lq             | 54.6                                       |                                            |                                                     | 212.6                                                 |
| 2-Chloronaphthalene             | c              | 55.2                                       |                                            |                                                     |                                                       |
| 1-Chlorooctane                  | lq             | − 291.3                                    |                                            |                                                     | 198.5                                                 |
| Chloropentafluoroacetone        | g              | − 1121.0                                   |                                            |                                                     |                                                       |
| Chloropentafluoroethane         | lq             |                                            |                                            |                                                     | 184.2                                                 |
|                                 | g              | − 1188.8                                   |                                            |                                                     |                                                       |
| 1-Chloropentane                 | lq             | − 213.2                                    |                                            |                                                     |                                                       |
|                                 | g              | − 175.0                                    | − 37.4                                     | 397.0                                               | 130.5                                                 |
| 3-Chlorophenol                  | c              | − 206.4                                    |                                            |                                                     |                                                       |
| 4-Chlorophenol                  | c              | − 197.9                                    |                                            |                                                     |                                                       |
| 1-Chloropropane                 | lq             | − 160.6                                    |                                            |                                                     | 132.2                                                 |
|                                 | g              | − 131.9                                    | − 50.7                                     | 319.1                                               | 84.6                                                  |
| 2-Chloropropane                 | lq             | − 172.1                                    |                                            |                                                     |                                                       |
|                                 | g              | − 144.9                                    | − 62.5                                     | 304.2                                               | 87.3                                                  |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                           | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 2-Chloro-1,3-propanediol            | lq             | -517.5                                     |                                            |                                                     |                                                       |
| 3-Chloro-1,2-propanediol            | lq             | -525.3                                     |                                            |                                                     |                                                       |
| 2-Chloropropanoic acid              | lq             | -522.5                                     |                                            |                                                     | 131.6                                                 |
| 3-Chloropropanoic acid              | c              | -549.3                                     |                                            |                                                     |                                                       |
| 2-Chloro-1-propene                  | g              | -21.0                                      |                                            |                                                     |                                                       |
| 3-Chloro-1-propene (allyl chloride) | lq             |                                            |                                            |                                                     | 125.1                                                 |
|                                     | g              | -0.63                                      | 43.6                                       | 306.7                                               | 75.4                                                  |
| <i>N</i> -Chlorosuccinimide         | c              | -358.1                                     |                                            |                                                     |                                                       |
| $\alpha$ -Chlorotoluene             | lq             | -32.6                                      |                                            |                                                     |                                                       |
| <i>o</i> -Chlorotoluene             | lq             |                                            |                                            |                                                     | 166.8                                                 |
| 2-Chloro-1,1,1-trifluoroethane      | g              |                                            |                                            | 326.4                                               | 154.6                                                 |
| Chlorotrifluoroethylene             | g              | -505.5                                     | -523.8                                     | 322.1                                               | 83.9                                                  |
| Chlorotrifluoromethane              | g              | -707.8                                     | -667.4                                     | 285.4                                               | 66.9                                                  |
| Chlorotrimethylsilane               | lq             | -384.1                                     |                                            |                                                     |                                                       |
| Chlorotrimethyromethane             | lq             | -27.1                                      |                                            |                                                     |                                                       |
|                                     | g              | 18.4                                       |                                            |                                                     |                                                       |
| Chrysene                            | c              | 145.3                                      |                                            |                                                     |                                                       |
| (-)-Cinchonidine                    | c              | 29.7                                       |                                            |                                                     |                                                       |
| Cinchonine                          | c              | 31.0                                       |                                            |                                                     |                                                       |
| <i>cis</i> -Cinnamic acid           | c              | -315.0                                     |                                            |                                                     |                                                       |
| <i>trans</i> -Cinnamic acid         | c              | -338.5                                     |                                            |                                                     |                                                       |
| Cinnamic anhydride                  | c              | -347.7                                     |                                            |                                                     |                                                       |
| Citric acid                         | c              | -1543.9                                    | -1236.4                                    | 166.2                                               |                                                       |
| Codeine monohydrate                 | c              | -632.6                                     |                                            |                                                     |                                                       |
| Creatine                            | c              | -537.2                                     |                                            |                                                     |                                                       |
| <i>o</i> -Cresol                    | c              | -204.6                                     |                                            | 165.4                                               | 154.6                                                 |
|                                     | lq             |                                            |                                            |                                                     | 233.6 <sup>40</sup>                                   |
|                                     | g              | -128.6                                     | 37.1                                       | 357.6                                               | 130.3                                                 |
| <i>m</i> -Cresol                    | lq             | -194.0                                     |                                            | 212.6                                               | 224.9                                                 |
|                                     | g              | -132.3                                     | -40.5                                      | 356.8                                               | 122.5                                                 |
| <i>p</i> -Cresol                    | c              | -199.3                                     |                                            | 167.3                                               | 150.2                                                 |
|                                     | lq             |                                            |                                            |                                                     | 221.0 <sup>40</sup>                                   |
|                                     | g              | -125.4                                     | -30.9                                      | 347.6                                               | 124.5                                                 |
| Cuban                               | c              | 541.3                                      |                                            |                                                     |                                                       |
| Cyanamide                           | c              | 58.8                                       |                                            |                                                     |                                                       |
| Cyanide (CN)                        | g              | 437.6                                      | 407.5                                      | 202.6                                               | 29.2                                                  |
| Cyanogen                            | g              | 306.7                                      | 297.2                                      | 241.9                                               | 56.9                                                  |
| Cyanogen bromide                    | g              | 140.5                                      | 165.3                                      | 248.3                                               | 46.9                                                  |
| Cyanogen chloride                   | g              | 138.0                                      | 131.0                                      | 236.2                                               | 45.0                                                  |
| Cyanogen fluoride                   | g              | -639.8                                     |                                            | 224.7                                               | 41.8                                                  |
| Cyanogen iodide                     | c              | 166.2                                      | 185.0                                      | 96.2                                                |                                                       |
|                                     | g              | 205.5                                      | 196.6                                      | 256.8                                               | 48.3                                                  |
| Cyclobutane                         | g              | 27.7                                       | 110.0                                      | 265.4                                               | 72.2                                                  |
| Cyclobutanecarbonitrile             | lq             | 103.0                                      |                                            |                                                     |                                                       |
| Cyclobutene                         | g              | 156.7                                      | 174.7                                      | 263.5                                               | 67.1                                                  |
| Cyclobutylamine                     | g              | 41.2                                       |                                            |                                                     |                                                       |
| Cyclododecane                       | c              | -306.6                                     |                                            |                                                     |                                                       |
| 1,3-Cycloheptadiene                 | g              | 94.3                                       |                                            |                                                     |                                                       |
| Cycloheptane                        | lq             | -156.6                                     | 54.1                                       | 242.6                                               | 123.1                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                               | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Cycloheptanone                          | lq             | − 299.4                                    |                                            |                                                     |                                                       |
| 1,3,5-Cycloheptatriene                  | lq             | 142.2                                      | 243.1                                      | 214.6                                               | 162.8                                                 |
| Cycloheptene                            | g              | − 9.2                                      |                                            |                                                     |                                                       |
| Cyclohexane                             | lq             | − 156.4                                    | 26.7                                       | 204.4                                               | 154.9                                                 |
|                                         | g              | − 123.4                                    | 31.8                                       | 298.3                                               | 106.3                                                 |
| cis-Cyclohexane-1,2-dicarboxylic acid   | c              | − 961.1                                    |                                            |                                                     |                                                       |
| trans-Cyclohexane-1,2-dicarboxylic acid | c              | − 970.7                                    |                                            |                                                     |                                                       |
| Cyclohexanethiol                        | lq             | − 140.7                                    |                                            | 255.6                                               | 192.6                                                 |
|                                         | g              | − 96.1                                     |                                            |                                                     |                                                       |
| Cyclohexanol                            | lq             | − 348.1                                    | − 133.3                                    | 199.6                                               | 208.2                                                 |
| Cyclohexanone                           | lq             | − 271.2                                    |                                            | 255.6                                               | 182.2                                                 |
|                                         | g              | − 226.1                                    | − 90.8                                     | 322.2                                               | 109.7                                                 |
| Cyclohexene                             | lq             | − 38.5                                     | 101.6                                      | 214.6                                               | 148.3                                                 |
| 1-Cyclohexenylmethanol                  | lq             | − 382.4                                    |                                            |                                                     |                                                       |
| Cyclohexylamine                         | lq             | − 147.7                                    |                                            |                                                     |                                                       |
| Cyclohexylbenzene                       | lq             | − 76.6                                     |                                            |                                                     | 261.3                                                 |
| Cyclohexylcyclohexane                   | lq             | − 329.3                                    |                                            |                                                     |                                                       |
| Cyclooctane                             | lq             | − 167.7                                    |                                            |                                                     |                                                       |
| Cyclooctanone                           | lq             | − 326.0                                    |                                            |                                                     |                                                       |
| 1,3,5,7-Cyclooctatetraene               | lq             | 254.5                                      | 358.6                                      | 220.3                                               | 184.0                                                 |
| Cyclooctene                             | lq             | − 74.0                                     |                                            |                                                     |                                                       |
| 1,3-Cyclopentadiene                     | g              | 134.3                                      | 179.3                                      | 267.8                                               |                                                       |
| Cyclopentane                            | lq             | − 105.1                                    | 36.4                                       | 204.3                                               | 128.9                                                 |
|                                         | g              | − 76.4                                     | 38.6                                       | 292.9                                               | 83.0                                                  |
| cis-1,2-Cyclopentanediol                | c              | − 484.9                                    |                                            |                                                     |                                                       |
| trans-1,2-Cyclopentanediol              | c              | − 489.9                                    |                                            |                                                     |                                                       |
| Cyclopentanethiol                       | lq             | − 89.5                                     | 46.8                                       | 256.9                                               | 165.2                                                 |
| Cyclopentanol                           | lq             | − 300.1                                    | − 127.8                                    | 206.3                                               | 184.1                                                 |
| Cyclopentanone                          | lq             | − 235.7                                    |                                            |                                                     | 154.5                                                 |
| Cyclopentene                            | lq             | 4.4                                        | 108.5                                      | 201.3                                               | 122.4                                                 |
|                                         | g              | 34.0                                       | 110.8                                      | 291.8                                               | 75.1                                                  |
| 1-Cyclopentenylmethanol                 | lq             | 34.3                                       |                                            |                                                     |                                                       |
| Cyclopentylamine                        | lq             | − 95.1                                     |                                            | 241.0                                               | 181.2                                                 |
| Cyclopropane                            | g              | 53.3                                       | 104.4                                      | 237.4                                               | 55.6                                                  |
| Cyclopropanecarbonitrile                | g              | 182.8                                      |                                            |                                                     |                                                       |
| Cyclopropene                            | g              | 277.1                                      | 286.3                                      | 223.3                                               |                                                       |
| Cyclopropylamine                        | lq             | 45.8                                       |                                            | 187.7                                               | 147.1                                                 |
|                                         | g              | 77.0                                       |                                            |                                                     |                                                       |
| Cyclopropylbenzene                      | lq             | 100.3                                      |                                            |                                                     |                                                       |
| (−)-Cysteine                            | c              | − 534.1                                    |                                            |                                                     |                                                       |
| (−)-Cystine                             | c              | − 1032.7                                   |                                            |                                                     |                                                       |
| Cytosine                                | c              | − 221.3                                    |                                            | 132.6                                               |                                                       |
| Decafluorobutane                        | lq             |                                            |                                            |                                                     | 127.2 <sup>20</sup>                                   |
| cis-Decahydronaphthalene                | lq             | − 219.4                                    | 68.9                                       | 265.0                                               | 232.0                                                 |
| trans-Decahydronaphthalene              | lq             | − 230.6                                    | 57.7                                       | 265.0                                               | 228.5                                                 |
| Decanal                                 | g              | − 330.9                                    | − 66.5                                     | 578.6                                               | 239.7                                                 |
| Decane                                  | lq             | − 300.9                                    | 17.5                                       | 425.5                                               | 314.4                                                 |
| Decanedioic acid                        | c              | − 1082.8                                   |                                            |                                                     |                                                       |
| 1,10-Decanediol                         | c              | − 693.5                                    |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                  | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 1-Decanenitrile                            | lq             | -158.4                                     |                                            |                                                     |                                                       |
| 1-Decanethiol                              | lq             | -276.5                                     |                                            | 476.1                                               | 350.4                                                 |
|                                            | g              | -211.5                                     | 61.4                                       | 610.1                                               | 255.6                                                 |
| Decanoic acid                              | c              | -713.7                                     |                                            |                                                     |                                                       |
| 1-Decanol                                  | lq             | -478.1                                     | -132.2                                     | 430.5                                               | 370.6                                                 |
| 1-Decene                                   | lq             | -173.8                                     | 105.0                                      | 425.0                                               | 300.8                                                 |
| 1-Decyne                                   | g              | 41.2                                       | 252.2                                      | 524.5                                               | 219.7                                                 |
| Deoxybenzoin                               | c              | -71.0                                      |                                            |                                                     |                                                       |
| Diacetamide                                | c              | -489.0                                     |                                            |                                                     |                                                       |
| Diacetyl peroxide                          | lq             | -535.3                                     |                                            |                                                     |                                                       |
| 1,2-Diallyl phthalate                      | lq             | -550.6                                     |                                            |                                                     |                                                       |
| 2,2'-Diaminodiethylamine                   | lq             |                                            |                                            |                                                     | 254 <sup>40</sup>                                     |
| 2,6-Diaminopyridine                        | c              | -6.5                                       |                                            |                                                     |                                                       |
| Diazomethane                               | g              | 192.5                                      | 217.8                                      | 242.8                                               | 52.5                                                  |
| Dibenz[ <i>de,kl</i> ]anthracene           | c              | 182.8                                      |                                            |                                                     |                                                       |
| 1,2-Dibenzoyl ethane                       | c              | -255.6                                     |                                            |                                                     |                                                       |
| <i>trans</i> -1,2-Dibenzoyl ethylene       | c              | -114.7                                     | 109.8                                      | 319.2                                               |                                                       |
| Dibenzoylmethane                           | c              | -223.5                                     |                                            |                                                     |                                                       |
| Dibenzoyl peroxide                         | c              | -369.6                                     |                                            |                                                     |                                                       |
| Dibenzyl                                   | c              | 44.1                                       | 260.0                                      | 269.4                                               | 255.2                                                 |
| Dibenzyl sulfide                           | c              | 99.0                                       |                                            |                                                     |                                                       |
| Dibenzyl sulfone                           | c              | -282.6                                     |                                            |                                                     |                                                       |
| 1,2-Dibromobutane                          | g              | -91.5                                      | -13.1                                      | 408.8                                               | 127.1                                                 |
| 1,3-Dibromobutane                          | lq             | -148.0                                     |                                            |                                                     |                                                       |
| 1,4-Dibromobutane                          | g              | -87.8                                      |                                            |                                                     |                                                       |
| 2,3-Dibromobutane                          | g              | -102.0                                     |                                            |                                                     |                                                       |
| Dibromochlorofluoromethane                 | g              | -231.8                                     | -223.4                                     | 342.8                                               | 82.4                                                  |
| Dibromochloromethane                       | g              | -20.9                                      | -18.8                                      | 327.7                                               | 69.2                                                  |
| 1,2-Dibromo-1-chloro-1,2,2-trifluoroethane | lq             | -691.7                                     |                                            |                                                     |                                                       |
|                                            | g              | -656.6                                     |                                            |                                                     |                                                       |
| 1,2-Dibromocycloheptane                    | lq             | -157.6                                     |                                            |                                                     |                                                       |
| 1,2-Dibromocyclohexane                     | lq             | -162.8                                     |                                            |                                                     |                                                       |
| 1,2-Dibromocyclooctane                     | lq             | -173.3                                     |                                            |                                                     |                                                       |
| Dibromodifluoroethane                      | g              | -36.9                                      |                                            | 327.7                                               | 80.8                                                  |
| Dibromodichloromethane                     | g              | -29.3                                      | -19.5                                      | 347.8                                               | 87.1                                                  |
| Dibromodifluoromethane                     | g              | -429.7                                     | -419.1                                     | 325.3                                               | 77.0                                                  |
| 1,1-Dibromoethane                          | lq             | -66.2                                      |                                            |                                                     |                                                       |
| 1,2-Dibromoethane                          | lq             | -79.2                                      | -20.9                                      | 223.3                                               | 136.0                                                 |
|                                            | g              | -37.5                                      |                                            |                                                     |                                                       |
| <i>cis</i> -1,2-Dibromoethylene            | g              |                                            |                                            | 313.3                                               | 68.8                                                  |
| <i>trans</i> -1,2-Dibromoethylene          | g              |                                            |                                            | 313.5                                               | 70.3                                                  |
| Dibromofluoromethane                       | g              | -223.4                                     | -221.1                                     | 316.8                                               | 65.1                                                  |
| Dibromomethane                             | lq             |                                            |                                            |                                                     | 105.3                                                 |
|                                            | g              | -14.8                                      | -16.2                                      | 293.2                                               | 54.7                                                  |
| 1,3-Dibromo-2-methylpropane                | g              | -137.6                                     |                                            |                                                     |                                                       |
| 1,3-Dibromotetrafluoroethane               | lq             | -817.7                                     |                                            |                                                     |                                                       |
|                                            | g              | -789.1                                     |                                            |                                                     |                                                       |
| 1,2-Dibromopropane                         | lq             |                                            |                                            |                                                     | 160.0                                                 |
|                                            | g              | -71.5                                      | -17.7                                      | 376.1                                               | 102.8                                                 |
| 1,2-Dibromotetrafluoroethane               | lq             |                                            |                                            |                                                     | 180.3                                                 |



**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                          | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Dibutoxymethane                    | lq             | − 549.4                                    |                                            |                                                     |                                                       |
| Dibutylamine                       | lq             | − 206.0                                    |                                            |                                                     | 292.9                                                 |
| Dibutyl disulfide                  | g              | − 160.6                                    | 53.9                                       | 572.8                                               | 231.1                                                 |
| Di- <i>tert</i> -butyl disulfide   | lq             | − 255.2                                    |                                            |                                                     |                                                       |
| Dibutyl ether                      | lq             | − 377.9                                    |                                            |                                                     | 278.2                                                 |
|                                    | g              | − 332.8                                    | − 88.5                                     | 500.4                                               | 204.0                                                 |
| Di- <i>sec</i> -butyl ether        | lq             | − 401.5                                    |                                            |                                                     |                                                       |
|                                    | g              | − 360.9                                    |                                            |                                                     |                                                       |
| Di- <i>tert</i> -butyl ether       | lq             | − 399.6                                    |                                            |                                                     | 276.1                                                 |
|                                    | g              | − 362.0                                    |                                            |                                                     |                                                       |
| Dibutylmercury                     | lq             | − 97.9                                     |                                            |                                                     |                                                       |
| Dibutyl peroxide                   | lq             | − 380.7                                    |                                            |                                                     |                                                       |
| Dibutyl 1,2-phthalate              | c              | − 842.6                                    |                                            |                                                     | 498.0                                                 |
| Dibutyl sulfate                    | lq             | − 904.6                                    |                                            |                                                     |                                                       |
| Dibutyl sulfide                    | lq             | − 220.7                                    | 32.2                                       | 405.1                                               | 284.3                                                 |
| Di- <i>tert</i> -butyl sulfide     | lq             | − 232.4                                    |                                            |                                                     |                                                       |
| Dibutyl sulfite                    | lq             | − 693.1                                    |                                            |                                                     |                                                       |
| Dibutyl sulfone                    | c              | − 610.2                                    |                                            |                                                     |                                                       |
| Dichloroacetic acid                | lq             | − 496.3                                    |                                            |                                                     |                                                       |
| ionized                            | aq             | − 507.1                                    |                                            |                                                     |                                                       |
| Dichloroacetyl chloride            | lq             | − 280.4                                    |                                            |                                                     |                                                       |
| 1,2-Dichlorobenzene                | lq             | − 17.5                                     |                                            |                                                     | 162.4                                                 |
|                                    | g              | 30.2                                       | 82.7                                       | 341.5                                               | 113.5                                                 |
| 1,3-Dichlorobenzene                | lq             | − 20.7                                     |                                            |                                                     | 171                                                   |
|                                    | g              | 25.7                                       | 78.6                                       | 343.5                                               | 113.8                                                 |
| 1,4-Dichlorobenzene                | c              | − 42.3                                     |                                            |                                                     |                                                       |
|                                    | lq             |                                            |                                            | 175.4                                               | 147.8                                                 |
|                                    | g              | 22.5                                       | 77.2                                       | 336.7                                               | 113.9                                                 |
| Dichlorodifluoromethane            | lq             |                                            |                                            |                                                     | 117.2                                                 |
|                                    | g              | − 477.4                                    | − 439.4                                    | 300.8                                               | 72.3                                                  |
| 1,3-Dichlorobutane                 | g              | − 195.0                                    |                                            |                                                     |                                                       |
| 1,4-Dichlorobutane                 | g              | − 183.4                                    |                                            |                                                     |                                                       |
| Dichlorodimethylsilane             | g              | − 461.1                                    |                                            | 335.4                                               | 101.1                                                 |
| Dichlorodiphenylsilane             | lq             | − 278.2                                    |                                            |                                                     |                                                       |
| 1,1-Dichloroethane                 | lq             | − 158.4                                    |                                            |                                                     | 126.3                                                 |
|                                    | g              | − 127.7                                    | − 73.8                                     | 305.1                                               | 76.2                                                  |
| 1,2-Dichloroethane                 | lq             | − 167.4                                    |                                            |                                                     | 128.4                                                 |
|                                    | g              | − 126.4                                    | − 73.9                                     | 308.4                                               | 78.7                                                  |
| 1,1-Dichloroethylene               | lq             | − 23.9                                     |                                            |                                                     | 111.3                                                 |
|                                    | g              | 2.8                                        | 25.4                                       | 289.1                                               | 67.0                                                  |
| <i>cis</i> -1,2-Dichloroethylene   | g              | 4.6                                        | 24.4                                       | 289.5                                               | 65.1                                                  |
| <i>trans</i> -1,2-Dichloroethylene | lq             | − 23.1                                     |                                            |                                                     | 116.8                                                 |
|                                    | g              | 5.0                                        | 28.6                                       | 289.9                                               | 66.7                                                  |
| Dichlorofluoromethane              | g              | − 283.0                                    | − 253.0                                    | 293.1                                               | 61.0                                                  |
| 1,1-Dichloro-1-fluoroethane        | g              |                                            |                                            | 320.2                                               | 88.7                                                  |
| 1,1-Dichlorofluoroethylene         | g              |                                            |                                            | 313.9                                               | 76.5                                                  |
| 1,1-Dichlorofluoromethane          | lq             |                                            |                                            |                                                     | 112.6                                                 |
| Dichloromethane                    | lq             | − 124.2                                    |                                            | 177.8                                               | 101.2                                                 |
|                                    | g              | − 95.4                                     | − 68.9                                     | 270.3                                               | 51.0                                                  |
| Dichloropentadienylnon             | c              | 141.0                                      |                                            |                                                     |                                                       |
| 1,2-Dichloropropane                | lq             | − 198.8                                    |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                          | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
|                                    | g              | -162.8                                     | -83.1                                      | 354.8                                               | 98.2                                                  |
| 1,3-Dichloropropane                | g              | -159.2                                     | -82.6                                      | 367.2                                               | 99.6                                                  |
| 2,2-Dichloropropane                | g              | -173.2                                     | -84.6                                      | 326.0                                               | 105.9                                                 |
| 1,3-Dichloro-2-propanol            | lq             | -385.4                                     |                                            |                                                     |                                                       |
| 2,3-Dichloro-1-propanol            | lq             | -381.3                                     |                                            |                                                     |                                                       |
| 2,3-Dichloropropene                | lq             | -73.3                                      |                                            |                                                     |                                                       |
| 1,2-Dichlorotetrafluoromethane     | lq             |                                            |                                            |                                                     | 164.2                                                 |
|                                    | g              | -916.3                                     |                                            |                                                     |                                                       |
| 2,2-Dichlorotetrafluoroethane      | lq             | -960.2                                     |                                            |                                                     | 111.7                                                 |
| 2,2-Dichloro-1,1,1-trifluoroethane | g              |                                            |                                            | 352.8                                               | 102.5                                                 |
| Dicyanoacetylene                   | lq             | 500.4                                      |                                            |                                                     |                                                       |
| Dicyanobenzene                     | c              | 275.4                                      |                                            |                                                     |                                                       |
| 1,4-Dicyanobutane                  | lq             | 85.1                                       |                                            |                                                     | 128.7                                                 |
| 1,4-Dicyano-2-butyne               | c              | 366.5                                      |                                            |                                                     |                                                       |
| Dicyanodiamide                     | c              | 22.6                                       | 179.5                                      | 129.3                                               | 118.8                                                 |
| Dicyclopentadiene                  | c              | 116.7                                      |                                            |                                                     |                                                       |
| Diethanolamine                     | c              | -493.8                                     |                                            |                                                     |                                                       |
|                                    | lq             |                                            |                                            |                                                     | 233.5 <sup>30</sup>                                   |
| 1,1-Diethoxyethane                 | lq             | -491.4                                     |                                            |                                                     | 238.0                                                 |
| 1,2-Diethoxyethane                 | lq             | -451.4                                     |                                            |                                                     | 259.4                                                 |
| Diethoxymethane                    | lq             | -450.4                                     |                                            |                                                     |                                                       |
| 1,3-Diethoxypropane                | lq             | -482.1                                     |                                            |                                                     |                                                       |
| 2,2-Diethoxypropane                | lq             | -538.5                                     |                                            |                                                     |                                                       |
| Diethylamine                       | lq             | -103.7                                     |                                            |                                                     | 169.2                                                 |
|                                    | g              | -72.2                                      | 72.1                                       | 352.2                                               | 115.7                                                 |
| Diethylamine hydrochloride         | c              | -358.6                                     |                                            |                                                     |                                                       |
| Diethylbarbituric acid (veronal)   | c              | -747.7                                     |                                            |                                                     |                                                       |
| 1,2-Diethylbenzene                 | g              | -19.0                                      | 141.1                                      | 434.3                                               | 182.6                                                 |
| 1,3-Diethylbenzene                 | g              | -21.8                                      | 136.7                                      | 439.3                                               | 176.9                                                 |
| 1,4-Diethylbenzene                 | g              | -22.3                                      | 137.9                                      | 434.0                                               | 176.2                                                 |
| Diethyl carbonate                  | lq             | -681.5                                     |                                            |                                                     | 212.4                                                 |
| cis-1,2-Diethylcyclopropane        | lq             | -79.9                                      |                                            |                                                     |                                                       |
| trans-1,2-Diethylcyclopropane      | lq             | 83.3                                       |                                            |                                                     |                                                       |
| Diethyl disulfide                  | lq             | -120.0                                     | 9.5                                        | 269.3                                               | 171.4                                                 |
|                                    | g              | -79.4                                      | 22.3                                       | 414.5                                               | 141.3                                                 |
| Diethylenediamine                  | c              | -13.4                                      | 240.2                                      | 85.8                                                |                                                       |
| Diethylene glycol                  | lq             | -628.5                                     |                                            |                                                     | 244.8                                                 |
|                                    | g              | -571.1                                     |                                            | 441.0                                               | 135.1                                                 |
| Diethylene glycol dibutyl ether    | lq             |                                            |                                            |                                                     | 452 <sup>20</sup>                                     |
| Diethylene glycol diethyl ether    | lq             |                                            |                                            |                                                     | 341.4 <sup>15</sup>                                   |
| Diethylene glycol dimethyl ether   | lq             |                                            |                                            |                                                     | 274.1                                                 |
| Diethylene glycol monoethyl ether  | lq             |                                            |                                            |                                                     | 301.0                                                 |
| Diethylene glycol monomethyl ether | lq             |                                            |                                            |                                                     | 271.1                                                 |
| Diethyl ether                      | lq             | -279.5                                     | -116.7                                     | 172.4                                               | 172.6                                                 |
|                                    | g              | -252.1                                     | -122.3                                     | 342.7                                               | 119.5                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                      | Physical State | $\Delta_f H^\circ$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $S^\circ$<br>$\text{J}\cdot\text{deg}^{-1}\cdot\text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J}\cdot\text{deg}^{-1}\cdot\text{mol}^{-1}$ |
|------------------------------------------------|----------------|-------------------------------------------------------|-------------------------------------------------------|-----------------------------------------------------------------|-------------------------------------------------------------------|
| Di-2-ethylhexyl phthalate                      | lq             |                                                       |                                                       |                                                                 | 704.7                                                             |
| Diethyl malonate                               | lq             | − 805.5                                               |                                                       |                                                                 | 260.7                                                             |
| Diethylmercury                                 | lq             | 30.1                                                  |                                                       |                                                                 | 182.8                                                             |
| Diethyl oxalate                                | lq             | − 805.5                                               |                                                       |                                                                 |                                                                   |
| 3,3-Diethylpentane                             | lq             | − 275.4                                               |                                                       |                                                                 | 278.2                                                             |
| Diethyl peroxide                               | lq             | − 223.3                                               |                                                       |                                                                 |                                                                   |
| Diethyl 1,2-phthalate                          | lq             | − 776.6                                               |                                                       | 425.1                                                           | 366.1                                                             |
| Diethyl selenide                               | lq             | − 96.2                                                |                                                       |                                                                 |                                                                   |
| Diethyl sulfate                                | lq             | − 813.2                                               |                                                       |                                                                 |                                                                   |
| Diethyl sulfide                                | lq             | − 119.4                                               |                                                       | 269.3                                                           | 171.4                                                             |
|                                                | g              | − 83.6                                                | 17.8                                                  | 368.0                                                           | 117.0                                                             |
| Diethyl sulfite                                | lq             | − 600.7                                               |                                                       |                                                                 |                                                                   |
| Diethyl sulfone                                | c              | − 515.5                                               |                                                       |                                                                 |                                                                   |
| Diethyl sulfoxide                              | lq             | − 268.0                                               |                                                       |                                                                 |                                                                   |
| <i>N,N</i> -Diethylurea                        | c              | − 372.2                                               |                                                       |                                                                 |                                                                   |
| Diethylzinc                                    | lq             | 16.7                                                  |                                                       |                                                                 |                                                                   |
| 1,2-Difluorobenzene                            | lq             | − 330.0                                               |                                                       | 222.6                                                           | 159.0                                                             |
|                                                | g              | − 293.8                                               | − 242.0                                               | 321.9                                                           | 106.5                                                             |
| 1,3-Difluorobenzene                            | lq             | − 343.9                                               |                                                       | 223.8                                                           | 159.1                                                             |
|                                                | g              | − 309.2                                               | − 257.0                                               | 320.4                                                           | 106.3                                                             |
| 1,4-Difluorobenzene                            | lq             | − 342.3                                               |                                                       |                                                                 | 157.5                                                             |
|                                                | g              | − 306.7                                               | − 252.8                                               | 315.6                                                           | 106.9                                                             |
| 2,2'-Difluorobiphenyl                          | c              | − 295.9                                               |                                                       |                                                                 |                                                                   |
| 4,4'-Difluorobiphenyl                          | c              | − 296.5                                               |                                                       |                                                                 |                                                                   |
| 1,1-Difluoroethane                             | lq             |                                                       |                                                       |                                                                 | 118.4                                                             |
|                                                | g              | − 497.0                                               | − 443.0                                               | 282.4                                                           | 67.8                                                              |
| 1,1-Difluoroethylene                           | g              | − 335.0                                               | − 321.5                                               | 266.2                                                           | 60.1                                                              |
| Difluoromethane                                | g              | − 452.2                                               | − 425.4                                               | 246.6                                                           | 42.9                                                              |
| 9,10-Dihydroanthracene                         | c              | 66.4                                                  |                                                       |                                                                 |                                                                   |
| 1,2-Dihydronaphthalene                         | lq             | 71.5                                                  |                                                       |                                                                 |                                                                   |
| 1,4-Dihydronaphthalene                         | lq             | 84.2                                                  |                                                       |                                                                 |                                                                   |
| Dihydro-2 <i>H</i> -pyran                      | lq             | − 157.4                                               |                                                       |                                                                 |                                                                   |
| 5,12-Dihydrotetracene                          | c              | 106.4                                                 |                                                       |                                                                 |                                                                   |
| 2,3-Dihydrothiophene                           | lq             | 52.9                                                  |                                                       |                                                                 |                                                                   |
|                                                | g              | 90.7                                                  | 133.5                                                 | 303.5                                                           | 79.8                                                              |
| 2,5-Dihydrothiophene                           | g              | 86.9                                                  | 131.6                                                 | 297.1                                                           | 83.3                                                              |
| 2,5-Dihydrothiophene-1,1-dioxide               | c              | 318.9                                                 |                                                       |                                                                 |                                                                   |
| 2',4-Dihydroxyacetophenone                     | c              | − 573.6                                               |                                                       |                                                                 |                                                                   |
| 1,2-Dihydroxybenzene (pyrocatechol)            | c              | − 354.1                                               | − 210.0                                               | 150.2                                                           | 132.2                                                             |
| 1,3-Dihydroxybenzene                           | c              | − 368.0                                               | − 209.2                                               | 147.7                                                           | 131.0                                                             |
| 1,4-Dihydroxybenzene ( <i>p</i> -hydroquinone) | c              | − 364.5                                               | − 207.0                                               | 140.2                                                           | 136.0                                                             |
| Dihydroxymalonic acid                          | c              | − 1216.3                                              |                                                       |                                                                 |                                                                   |
| 2,4-Dihydroxy-5-methylpyrimidine               | c              | − 468.2                                               |                                                       |                                                                 |                                                                   |
| 2,4-Dihydroxy-6-methylpyrimidine               | c              | − 456.9                                               |                                                       |                                                                 |                                                                   |
| Diiodoacetylene                                | g              |                                                       |                                                       | 313.1                                                           | 70.3                                                              |
| 1,2-Diiodobenzene                              | c              | 172.4                                                 |                                                       |                                                                 |                                                                   |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                     | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 1,3-Diiodobenzene                             | c              | 187.0                                      |                                            |                                                     |                                                       |
| 1,4-Diiodobenzene                             | lq             | -30.0                                      |                                            |                                                     |                                                       |
|                                               | c              | 160.7                                      |                                            |                                                     |                                                       |
| 1,2-Diiodoethane                              | g              | 75.0                                       | 78.5                                       | 348.5                                               | 82.3                                                  |
| Diiodomethane                                 | lq             | 66.9                                       | 90.4                                       | 174.1                                               | 134.0                                                 |
|                                               | g              | 119.5                                      | 95.8                                       | 309.7                                               | 57.7                                                  |
| 1,2-Diiodopropane                             | g              | 35.6                                       |                                            |                                                     |                                                       |
| 1,3-Diiodopropane                             | lq             | -9.0                                       |                                            |                                                     |                                                       |
| Diisobutylamine                               | lq             | -218.5                                     |                                            |                                                     |                                                       |
| Diisopentyl ether                             | lq             |                                            |                                            |                                                     | 379 <sup>100</sup>                                    |
| Diisopropylamine                              | lq             | -178.5                                     |                                            |                                                     |                                                       |
| Diisopropyl ether                             | lq             | -351.5                                     |                                            |                                                     | 216.8                                                 |
|                                               | g              | -319.2                                     | -121.9                                     | 390.2                                               | 158.3                                                 |
| Diisopropylmercury                            | lq             | -13.0                                      |                                            |                                                     |                                                       |
| Diisopropyl sulfide                           | lq             | -181.6                                     |                                            | 313.0                                               | 232.0                                                 |
|                                               | g              | -142.1                                     | 27.1                                       | 415.5                                               | 169.2                                                 |
| Diketene                                      | lq             | -233.1                                     |                                            |                                                     |                                                       |
| 1,2-Dimethoxybenzene                          | lq             | -290.4                                     |                                            |                                                     |                                                       |
| 1,1-Dimethoxybutane                           | lq             | -468.1                                     |                                            |                                                     |                                                       |
| 2,2-Dimethoxybutane                           | lq             | -485.1                                     |                                            |                                                     |                                                       |
| 1,1-Dimethoxyethane                           | lq             | -420.2                                     |                                            |                                                     |                                                       |
| 1,2-Dimethoxyethane                           | lq             | -376.7                                     |                                            |                                                     | 193.3                                                 |
| Dimethoxymethane                              | lq             | -377.8                                     |                                            | 244.0                                               | 161.3                                                 |
| 1,1-Dimethoxypentane                          | lq             | -494.6                                     |                                            |                                                     |                                                       |
| 2,2-Dimethoxypentane                          | lq             | -509.2                                     |                                            |                                                     |                                                       |
| 1,1-Dimethoxypropane                          | lq             | -443.3                                     |                                            |                                                     |                                                       |
| 2,2-Dimethoxypropane                          | lq             | -459.0                                     |                                            |                                                     |                                                       |
| 1,1-Dimethoxy-2-methyl-<br>propane            | lq             | -476.2                                     |                                            |                                                     |                                                       |
| <i>N,N</i> -Dimethylacetamide                 | lq             | -278.3                                     |                                            |                                                     | 175.6                                                 |
| Dimethylamine                                 | lq             | -43.9                                      | 70.0                                       | 182.3                                               | 137.7                                                 |
|                                               | g              | -18.5                                      | 68.5                                       | 273.0                                               | 70.7                                                  |
| 4-(Dimethylamino)benz-<br>aldehyde            | c              | -137.6                                     |                                            |                                                     |                                                       |
| Dimethylaminomethanol                         | lq             | -253.6                                     |                                            |                                                     |                                                       |
| <i>N,N</i> -Dimethylaminotri-<br>methylsilane | lq             | -279.5                                     |                                            |                                                     |                                                       |
| <i>N,N</i> -Dimethylaniline                   | lq             | 47.7                                       |                                            |                                                     | 214.6 <sup>29</sup>                                   |
| 2,6-Dimethylaniline                           | lq             |                                            |                                            |                                                     | 238.9                                                 |
| 2,3-Dimethylbenzoic acid                      | c              | -450.4                                     |                                            |                                                     |                                                       |
| 2,4-Dimethylbenzoic acid                      | c              | -458.5                                     |                                            |                                                     |                                                       |
| 2,5-Dimethylbenzoic acid                      | c              | -456.1                                     |                                            |                                                     |                                                       |
| 2,6-Dimethylbenzoic acid                      | c              | -440.7                                     |                                            |                                                     |                                                       |
| 3,4-Dimethylbenzoic acid                      | c              | -468.8                                     |                                            |                                                     |                                                       |
| 3,5-Dimethylbenzoic acid                      | c              | -466.4                                     |                                            |                                                     |                                                       |
| 3,3'-Dimethylbiphenyl                         | lq             | 20.0                                       |                                            |                                                     |                                                       |
| 2,2-Dimethylbutane                            | lq             | -213.8                                     |                                            | 272.5                                               | 191.9                                                 |
|                                               | g              | -186.1                                     | -9.2                                       | 358.2                                               | 141.9                                                 |
| 2,3-Dimethylbutane                            | lq             | -207.4                                     |                                            | 287.8                                               | 189.7                                                 |
|                                               | g              | -178.3                                     | -4.1                                       | 365.8                                               | 140.5                                                 |
| 3,3-Dimethyl-2-butanone                       | lq             | -328.6                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                      | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 2,3-Dimethyl-1-butene          |                | -62.6                                      | 79.0                                       | 365.6                                               | 143.5                                                 |
| 2,3-Dimethyl-2-butene          | lq             | -101.4                                     |                                            | 270.2                                               | 174.7                                                 |
|                                | g              | -68.2                                      | 76.1                                       | 364.6                                               | 123.6                                                 |
| 3,3-Dimethyl-1-butene          | g              | -60.5                                      | 98.2                                       | 343.8                                               | 126.5                                                 |
| 2,3-Dimethyl-2-butenic acid    | c              | -455.6                                     |                                            |                                                     |                                                       |
| Dimethylcadmium                | lq             | 63.6                                       | 139.3                                      | 201.9                                               | 132.0                                                 |
| 1,1-Dimethylcyclohexane        | lq             | -218.7                                     | 26.5                                       | 267.2                                               | 209.2                                                 |
|                                | g              | -180.9                                     | 35.2                                       | 365.0                                               | 154.4                                                 |
| cis-1,2-Dimethylcyclohexane    | lq             | -211.8                                     |                                            | 274.1                                               | 210.2                                                 |
|                                | g              | -172.1                                     | 41.2                                       | 374.5                                               | 165.5                                                 |
| trans-1,2-Dimethylcyclohexane  | lq             | -218.2                                     |                                            | 273.2                                               | 209.4                                                 |
|                                | g              | -180.0                                     | 34.5                                       | 370.9                                               | 159.0                                                 |
| cis-1,3-Dimethylcyclohexane    | lq             | -222.9                                     |                                            | 272.6                                               | 209.4                                                 |
|                                | g              | -184.6                                     | 29.8                                       | 370.5                                               | 157.3                                                 |
| trans-1,3-Dimethylcyclohexane  | lq             | -215.7                                     |                                            | 276.3                                               | 212.8                                                 |
|                                | g              | -176.5                                     | 36.3                                       | 376.2                                               | 157.3                                                 |
| cis-1,4-Dimethylcyclohexane    | lq             | -215.6                                     |                                            | 271.1                                               | 212.1                                                 |
|                                | g              | -176.6                                     | 38.0                                       | 370.5                                               | 157.3                                                 |
| trans-1,4-Dimethylcyclohexane  | lq             | -222.4                                     |                                            | 268.0                                               | 210.2                                                 |
|                                | g              | -184.5                                     | 31.7                                       | 364.8                                               | 157.7                                                 |
| 1,1-Dimethylcyclopentane       | g              | -138.2                                     | 39.0                                       | 359.3                                               | 133.3                                                 |
| cis-1,2-Dimethylcyclopentane   | lq             | -165.3                                     |                                            | 269.2                                               |                                                       |
|                                | g              | -129.5                                     | 45.7                                       | 366.1                                               | 134.14                                                |
| trans-1,2-Dimethylcyclopentane | g              | -136.6                                     | 38.4                                       | 366.8                                               | 134.5                                                 |
| cis-1,3-Dimethylcyclopentane   | g              | -135.9                                     | 39.2                                       | 366.8                                               | 134.5                                                 |
| trans-1,3-Dimethylcyclopentane | g              | -133.6                                     | 41.5                                       | 366.8                                               | 134.5                                                 |
| 1,1-Dimethylcyclopropane       | lq             | -33.3                                      |                                            |                                                     |                                                       |
| cis-1,2-Dimethylcyclopropane   | lq             | -26.3                                      |                                            |                                                     |                                                       |
| trans-1,2-Dimethylcyclopropane | lq             | -30.7                                      |                                            |                                                     |                                                       |
| cis-2,4-Dimethyl-1,3-dioxane   | lq             | -465.2                                     |                                            |                                                     |                                                       |
| 4,5-Dimethyl-1,3-dioxane       | lq             | -451.6                                     |                                            |                                                     |                                                       |
| 5,5-Dimethyl-1,3-dioxane       | lq             | -461.3                                     |                                            |                                                     |                                                       |
| 4,4'-Dimethyldiphenylamine     | c              | -11.72                                     |                                            |                                                     |                                                       |
| Dimethyl disulfide             | lq             | -62.6                                      | 7.0                                        | 235.4                                               | 146.1                                                 |
| Dimethyl ether                 | g              | -184.1                                     | -112.6                                     | 266.4                                               | 64.4                                                  |
| N,N-Dimethylformamide          | lq             | -239.3                                     |                                            |                                                     | 150.6                                                 |
| Dimethyl fumarate              | lq             | -729.3                                     |                                            |                                                     |                                                       |
| Dimethylglyoxime               | c              | -199.7                                     |                                            |                                                     |                                                       |
| 2,2-Dimethylheptane            | lq             | -288.2                                     |                                            |                                                     |                                                       |
| 2,6-Dimethyl-4-heptanone       | lq             | -408.5                                     |                                            |                                                     | 297.3                                                 |
| 2,2-Dimethylhexane             | lq             | -261.9                                     | 3.0                                        | 331.9                                               |                                                       |
| 2,3-Dimethylhexane             | lq             | -252.6                                     | 9.1                                        | 342.7                                               |                                                       |
| 2,4-Dimethylhexane             | lq             | -257.0                                     | 3.7                                        | 345.7                                               |                                                       |
| 2,5-Dimethylhexane             | lq             | -260.4                                     | 2.5                                        | 338.7                                               | 249.2                                                 |
| 3,3-Dimethylhexane             | lq             | -257.5                                     | 5.2                                        | 339.4                                               | 246.6                                                 |
| 3,4-Dimethylhexane             | lq             | -251.8                                     | 8.5                                        | 347.2                                               |                                                       |
| Dimethyl hexanedioate          | lq             | -886.6                                     |                                            |                                                     |                                                       |
| cis-2,2-Dimethyl-3-hexene      | lq             | -126.4                                     |                                            |                                                     |                                                       |
| trans-2,2-Dimethyl-3-hexene    | lq             | -144.9                                     |                                            |                                                     |                                                       |
| cis-2,5-Dimethyl-3-hexene      | lq             | -151.0                                     |                                            |                                                     |                                                       |
| trans-2,5-Dimethyl-3-hexene    | lq             | -159.2                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                          | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 5,5-Dimethylhydantoin                              | c              | -533.3                                     |                                            |                                                     |                                                       |
| 1,1-Dimethylhydrazine                              | lq             | 48.9                                       | 206.7                                      | 198.0                                               | 164.1                                                 |
| 1,2-Dimethylhydrazine                              | lq             | 52.7                                       | 212.6                                      | 199.2                                               | 171.0                                                 |
| 3,5-Dimethylisoxazole                              | lq             | -63.2                                      |                                            |                                                     |                                                       |
| Dimethyl maleate                                   | lq             | -703.8                                     |                                            |                                                     | 263.2                                                 |
| Dimethylmaleic anhydride                           | c              | -581.6                                     |                                            |                                                     |                                                       |
| Dimethyl malonate                                  | lq             | -795.8                                     |                                            |                                                     |                                                       |
| Dimethylmercury                                    | lq             | 59.8                                       | 140.3                                      | 209.0                                               |                                                       |
|                                                    | g              | 94.4                                       | 146.1                                      | 306.0                                               | 83.3                                                  |
| 6,6-Dimethyl-2-methylene-<br>bicyclo[3.1.1]heptane | lq             | -7.7                                       |                                            |                                                     |                                                       |
| Dimethyl oxalate                                   | lq             | -756.3                                     |                                            |                                                     |                                                       |
| 2,2-Dimethylpentane                                | lq             | -238.3                                     |                                            | 300.3                                               | 221.1                                                 |
|                                                    | g              | -205.9                                     | 0.1                                        | 392.9                                               | 166.0                                                 |
| 2,3-Dimethylpentane                                | lq             | -233.1                                     |                                            |                                                     | 218.3                                                 |
|                                                    | g              | -198.9                                     | 0.7                                        | 414.0                                               | 166.0                                                 |
| 2,4-Dimethylpentane                                | lq             | -234.6                                     |                                            | 303.2                                               | 224.2                                                 |
|                                                    | g              | -201.7                                     | 3.1                                        | 396.6                                               | 166.0                                                 |
| 3,3-Dimethylpentane                                | lq             | -234.2                                     |                                            |                                                     |                                                       |
|                                                    | g              | -201.2                                     | 2.6                                        | 399.7                                               | 166.0                                                 |
| Dimethyl pentanedioate                             | lq             | -205.9                                     |                                            |                                                     |                                                       |
| 2,4-Dimethyl-3-pentanone                           | lq             | -352.9                                     |                                            | 318.0                                               | 233.7                                                 |
|                                                    | g              | -311.5                                     |                                            |                                                     |                                                       |
| 2,4-Dimethyl-1-pentene                             | g              | -83.8                                      |                                            |                                                     |                                                       |
| 4,4-Dimethyl-1-pentene                             | g              | -81.6                                      |                                            |                                                     |                                                       |
| 2,4-Dimethyl-2-pentene                             | g              | -88.7                                      |                                            |                                                     |                                                       |
| cis-4,4-Dimethyl-2-pentene                         | g              | -72.6                                      |                                            |                                                     |                                                       |
| trans-4,4-Dimethyl-2-pentene                       | g              | -88.8                                      |                                            |                                                     |                                                       |
| 2,7-Dimethylphenanthrene                           | c              | 36.4                                       |                                            |                                                     |                                                       |
| 4,5-Dimethylphenanthrene                           | c              | 89.0                                       |                                            |                                                     |                                                       |
| 9,10-Dimethylphenanthrene                          | c              | 47.7                                       |                                            |                                                     |                                                       |
| 2,3-Dimethylphenol                                 | c              | -241.2                                     |                                            |                                                     | 206.9                                                 |
| 2,4-Dimethylphenol                                 | lq             | -228.7                                     |                                            |                                                     |                                                       |
| 2,5-Dimethylphenol                                 | c              | -246.6                                     |                                            |                                                     |                                                       |
| 2,6-Dimethylphenol                                 | c              | -237.4                                     |                                            |                                                     |                                                       |
| 3,4-Dimethylphenol                                 | c              | -242.3                                     |                                            |                                                     |                                                       |
| 3,5-Dimethylphenol                                 | c              | -244.4                                     |                                            |                                                     |                                                       |
| Dimethyl 1,2-phthalate                             | lq             | -678                                       |                                            |                                                     | 303.1                                                 |
| Dimethyl 1,3-phthalate                             | c              | -730.0                                     |                                            |                                                     |                                                       |
| Dimethyl 1,4-phthalate                             | c              | -732.6                                     |                                            |                                                     | 261.1                                                 |
| 2,2-Dimethylpropane                                | lq             |                                            |                                            |                                                     | 163.9 <sup>6</sup>                                    |
|                                                    | g              | -168.0                                     | -1.5                                       | 306.4                                               | 121.6                                                 |
| 2,2-Dimethylpropanenitrile                         | lq             | -39.8                                      |                                            | 232.0                                               | 179.4                                                 |
| 2,2-Dimethyl-1,3-propanediol                       | c              | -551.2                                     |                                            |                                                     |                                                       |
| 2,2-Dimethylpropanoic acid                         | lq             | -564.4                                     |                                            |                                                     |                                                       |
| 2,2-Dimethylpropanoic<br>anhydride                 | lq             | -779.9                                     |                                            |                                                     |                                                       |
| 2,2-Dimethyl-1-propanol                            | lq             | -399.4                                     |                                            |                                                     |                                                       |
| 2,3-Dimethylpyridine                               | lq             | 19.4                                       |                                            | 243.7                                               | 189.5                                                 |
| 2,4-Dimethylpyridine                               | lq             | 16.2                                       |                                            | 248.5                                               | 184.8                                                 |
| 2,5-Dimethylpyridine                               | lq             | 18.7                                       |                                            | 248.8                                               | 184.7                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                      | Physical State | $\Delta_f H^\circ$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $S^\circ$<br>$\text{J}\cdot\text{deg}^{-1}\cdot\text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J}\cdot\text{deg}^{-1}\cdot\text{mol}^{-1}$ |
|--------------------------------|----------------|-------------------------------------------------------|-------------------------------------------------------|-----------------------------------------------------------------|-------------------------------------------------------------------|
| 2,6-Dimethylpyridine           | lq             | 12.7                                                  |                                                       | 249.2                                                           | 185.2                                                             |
| 3,4-Dimethylpyridine           | lq             | 18.3                                                  |                                                       | 240.7                                                           | 191.8                                                             |
| 3,5-Dimethylpyridine           | lq             | 22.5                                                  |                                                       | 241.7                                                           | 184.5                                                             |
| Dimethyl succinate             | lq             | − 835.1                                               |                                                       |                                                                 |                                                                   |
| 2,2-Dimethylsuccinic acid      | c              | − 987.8                                               |                                                       |                                                                 |                                                                   |
| meso-2,3-Dimethylsuccinic acid | c              | − 977.5                                               |                                                       |                                                                 |                                                                   |
| Dimethyl sulfate               | lq             | − 735.5                                               |                                                       |                                                                 |                                                                   |
| Dimethyl sulfide               | lq             | − 65.4                                                |                                                       |                                                                 | 118.1                                                             |
|                                | g              | − 37.5                                                | 7.0                                                   | 285.9                                                           | 74.1                                                              |
| Dimethyl sulfite               | lq             | − 523.6                                               |                                                       |                                                                 |                                                                   |
| Dimethyl sulfone               | c              | − 450.1                                               | − 302.5                                               | 142.0                                                           |                                                                   |
|                                | lq             | − 373.1                                               | − 272                                                 |                                                                 |                                                                   |
|                                | g              |                                                       |                                                       | 310.6                                                           | 100.0                                                             |
| Dimethyl sulfoxide             | lq             | − 204.2                                               | − 99.2                                                | 188.3                                                           | 153.0                                                             |
| 1,5-Dimethyltetrazole          | c              | 188.7                                                 |                                                       |                                                                 |                                                                   |
| 2,2-Dimethylthiacyclopropane   | lq             | − 24.2                                                |                                                       |                                                                 |                                                                   |
| 5,5-Dimethyl-4-thia-1-hexene   | lq             | − 90.7                                                |                                                       |                                                                 |                                                                   |
| N,N-Dimethylurea               | c              | − 319.1                                               |                                                       |                                                                 |                                                                   |
| N,N'-Dimethylurea              | c              | − 312.1                                               |                                                       |                                                                 |                                                                   |
| Dimethylzinc                   | lq             | 23.4                                                  |                                                       | 201.6                                                           | 129.2                                                             |
| 2,3-Dinitroaniline             | c              | − 11.7                                                |                                                       |                                                                 |                                                                   |
| 2,4-Dinitroaniline             | c              | − 67.8                                                |                                                       |                                                                 |                                                                   |
| 2,5-Dinitroaniline             | c              | − 44.4                                                |                                                       |                                                                 |                                                                   |
| 2,6-Dinitroaniline             | c              | − 50.6                                                |                                                       |                                                                 |                                                                   |
| 3,4-Dinitroaniline             | c              | − 32.6                                                |                                                       |                                                                 |                                                                   |
| 3,5-Dinitroaniline             | c              | − 38.9                                                |                                                       |                                                                 |                                                                   |
| 2,4-Dinitroanisole             | c              | − 186.6                                               |                                                       |                                                                 |                                                                   |
| 2,6-Dinitroanisole             | c              | − 189.1                                               |                                                       |                                                                 |                                                                   |
| 1,2-Dinitrobenzene             | c              | − 1.8                                                 | 211.5                                                 | 216.3                                                           |                                                                   |
| 1,3-Dinitrobenzene             | c              | − 27.4                                                | 184.6                                                 | 220.9                                                           |                                                                   |
| 1,4-Dinitrobenzene             | c              | − 38.7                                                |                                                       |                                                                 |                                                                   |
| 1,1-Dinitroethane              | lq             | − 148.2                                               |                                                       |                                                                 |                                                                   |
| 1,2-Dinitroethane              | lq             | − 165.2                                               |                                                       |                                                                 |                                                                   |
| Dinitromethane                 | lq             | − 104.9                                               |                                                       |                                                                 |                                                                   |
|                                | g              | − 58.9                                                |                                                       |                                                                 |                                                                   |
| 1,5-Dinitronaphthalene         | c              | 30.5                                                  |                                                       |                                                                 |                                                                   |
| 2,4-Dinitro-1-naphthol         | c              | − 181.4                                               |                                                       |                                                                 |                                                                   |
| 2,4-Dinitrophenol              | c              | − 232.6                                               |                                                       |                                                                 |                                                                   |
| 2,6-Dinitrophenol              | c              | − 210.0                                               |                                                       |                                                                 |                                                                   |
| 1,1-Dinitropropane             | lq             | − 163.2                                               |                                                       |                                                                 |                                                                   |
| 1,3-Dinitropropane             | lq             | − 207.1                                               |                                                       |                                                                 |                                                                   |
| 2,2-Dinitropropane             | lq             | − 181.2                                               |                                                       |                                                                 |                                                                   |
| 2,4-Dinitroresorcinol          | c              | − 415.5                                               |                                                       |                                                                 |                                                                   |
| 2,4-Dinitrotoluene             | c              | − 71.6                                                |                                                       |                                                                 |                                                                   |
| 2,6-Dinitrotoluene             | c              | − 51.0                                                |                                                       |                                                                 |                                                                   |
| 1,3-Dioxane                    | lq             | − 379.7                                               |                                                       |                                                                 | 143.9                                                             |
| 1,4-Dioxane                    | lq             | − 353.9                                               | − 188.1                                               | 270.2                                                           | 153.6                                                             |
|                                | g              | − 315.8                                               | − 180.8                                               | 299.8                                                           | 94.1                                                              |
| 1,3-Dioxolane                  | lq             | − 333.5                                               |                                                       |                                                                 | 118.0                                                             |
|                                | g              | − 298.0                                               |                                                       |                                                                 |                                                                   |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                 | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 1,3-Dioxolan-2-one                        | c              | -581.6                                     |                                            |                                                     | 133.9 <sup>50</sup>                                   |
| 1,3-Dioxol-2-one                          | lq             | -459.9                                     |                                            |                                                     |                                                       |
| Dipentene                                 | lq             | -50.8                                      |                                            |                                                     | 249.4                                                 |
| Dipentyl ether                            | lq             |                                            |                                            |                                                     | 250                                                   |
| <i>N,N</i> -Diphenylacetamide             | c              | -43.1                                      |                                            |                                                     |                                                       |
| Diphenylacetylene                         | c              | 312.4                                      |                                            |                                                     | 225.9                                                 |
| Diphenylamine                             | c              | 130.6                                      |                                            |                                                     |                                                       |
| Diphenylboron bromide                     | lq             | -16.1                                      |                                            |                                                     |                                                       |
| <i>cis,cis</i> -1,4-Diphenylbutadiene     | c              | 198.8                                      |                                            |                                                     |                                                       |
| <i>trans,trans</i> -1,4-Diphenylbutadiene | c              | 178.8                                      |                                            |                                                     |                                                       |
| Diphenylbutadiyne                         | c              | 518.4                                      |                                            |                                                     |                                                       |
| 1,4-Diphenylbutane                        | c              | -9.9                                       |                                            |                                                     |                                                       |
| 1,4-Diphenyl-1,4-butanedione              | c              | -256.2                                     | 7.8                                        | 324.7                                               |                                                       |
| 1,4-Diphenyl-2-butene-1,4-dione           | c              | -114.7                                     | 111.5                                      | 319.2                                               |                                                       |
| Diphenyl carbonate                        | c              | -401.2                                     | -175.9                                     | 278.4                                               |                                                       |
| Diphenyl disulfide                        | c              | -148.5                                     |                                            |                                                     |                                                       |
| Diphenyl disulfone                        | c              | -643.2                                     |                                            |                                                     |                                                       |
| Diphenyleneimine                          | c              | 126.8                                      |                                            |                                                     |                                                       |
| 1,1-Diphenylethane                        | lq             | 48.7                                       | 245.1                                      | 335.9                                               |                                                       |
| 1,2-Diphenylethane                        | lq             | 51.5                                       | 67.2                                       | 270.3                                               |                                                       |
| Diphenylethanedione                       | c              | -154.0                                     |                                            |                                                     |                                                       |
| Diphenyl ether                            | c              | -32.1                                      |                                            | 233.9                                               | 216.6                                                 |
|                                           | lq             | -14.9                                      | 144.2                                      | 291.3                                               | 268.6                                                 |
| 1,1-Diphenylethylene                      | lq             | 172.4                                      |                                            |                                                     |                                                       |
| Diphenylethyne                            | c              | 312.4                                      |                                            |                                                     |                                                       |
| 6,6-Diphenylfulvene                       | c              | 197.4                                      |                                            |                                                     |                                                       |
| 1,2-Diphenylhydrazine                     | c              | 221.3                                      |                                            |                                                     |                                                       |
| Diphenylmercury                           | c              | 279.5                                      |                                            |                                                     |                                                       |
| Diphenylmethane                           | c              | 71.7                                       |                                            | 239.3                                               |                                                       |
|                                           | lq             | 89.7                                       | 276.9                                      |                                                     | 233.1                                                 |
| 1,3-Diphenyl-2-propanone                  | c              | -84.0                                      |                                            |                                                     |                                                       |
| Diphenyl sulfide                          | lq             | 163.4                                      |                                            |                                                     |                                                       |
| Diphenyl sulfone                          | c              | -225.0                                     |                                            |                                                     |                                                       |
| Diphenyl sulfoxide                        | c              | 9.7                                        |                                            |                                                     |                                                       |
| 1,3-Diphenylurea                          | c              | -122.6                                     |                                            |                                                     |                                                       |
| Dipropylamine                             | lq             | -156.1                                     |                                            |                                                     | 253.0 <sup>75</sup>                                   |
| Dipropyl disulfide                        | lq             | -171.3                                     | 19.1                                       | 373.6                                               |                                                       |
| Dipropyl ether                            | lq             | -328.8                                     |                                            | 323.9                                               | 221.6                                                 |
|                                           | g              | -292.9                                     | -105.6                                     | 422.5                                               | 158.3                                                 |
| Dipropylmercury                           | lq             | -20.9                                      |                                            |                                                     |                                                       |
| Dipropyl sulfate                          | lq             | -859.0                                     |                                            |                                                     |                                                       |
| Dipropyl sulfide                          | lq             | -171.5                                     |                                            |                                                     |                                                       |
|                                           | g              | -125.3                                     | 33.2                                       | 448.4                                               | 161.2                                                 |
| Dipropyl sulfite                          | lq             | -646.8                                     |                                            |                                                     |                                                       |
| Dipropyl sulfone                          | lq             | -548.2                                     |                                            |                                                     |                                                       |
| Dipropyl sulfoxide                        | lq             | -329.4                                     |                                            |                                                     |                                                       |
| 2,2'-Dipyridyl ketone                     | c              | -19.7                                      |                                            |                                                     |                                                       |
| 1,3-Dithiane                              | g              | -10.0                                      | 72.4                                       | 333.5                                               | 110.4                                                 |
| 1,2-Dithiolane                            | g              | 0.0                                        | 47.7                                       | 313.5                                               | 86.5                                                  |
| 1,3-Dithiolane                            | g              | 10.0                                       | 54.7                                       | 323.3                                               | 84.7                                                  |



**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Divinyl ether            | lq             | -39.8                                      |                                            |                                                     |                                                       |
|                          | g              | -13.6                                      |                                            |                                                     |                                                       |
| Divinyl sulfone          | lq             | -207.4                                     |                                            |                                                     |                                                       |
| Docosanoic acid          | c              | -983.0                                     |                                            |                                                     |                                                       |
| cis-13-Docosenic acid    | c              | -866.0                                     |                                            |                                                     |                                                       |
| trans-13-Docosenic acid  | c              | -960.7                                     |                                            |                                                     |                                                       |
| Dodecane                 | lq             | -350.9                                     | 28.1                                       | 490.6                                               | 376.0                                                 |
|                          | g              | -289.7                                     | 50.0                                       | 622.5                                               | 280.3                                                 |
| Dodecanedioic acid       | c              | -1130.0                                    |                                            |                                                     |                                                       |
| Dodecanoic acid          | c              | -774.6                                     |                                            |                                                     |                                                       |
|                          | lq             | -737.9                                     |                                            |                                                     | 404.3                                                 |
| 1-Dodecanol              | lq             | -528.5                                     |                                            |                                                     | 438.1                                                 |
| 1-Dodecene               | lq             | -226.2                                     |                                            | 484.8                                               | 360.7                                                 |
|                          | g              | -165.4                                     | 137.9                                      | 618.3                                               | 269.6                                                 |
| 1-Dodecyne               | g              | -0.04                                      | 268.6                                      | 602.4                                               | 265.4                                                 |
| Dulcitol                 | c              | -1346.8                                    |                                            |                                                     |                                                       |
| 1,2-Epoxybutane          | lq             | -168.9                                     |                                            | 230.9                                               | 147.0                                                 |
| Ergosterol               | c              | -789.9                                     |                                            |                                                     |                                                       |
| Ethane                   | g              | -84.0                                      | -32.0                                      | 229.1                                               | 52.5                                                  |
| Ethane-d <sub>6</sub>    | g              | -107.4                                     | -47.3                                      | 244.5                                               | 64.6                                                  |
| 1,2-Ethanediamine        | lq             | -63.0                                      |                                            | 209.2                                               | 172.6                                                 |
| 1,2-Ethanediol           | lq             | -455.3                                     | -323.2                                     | 163.2                                               | 149.3                                                 |
|                          | g              | -392.2                                     | -304.5                                     | 303.8                                               | 82.7                                                  |
| Ethanedithioamide        | c              | -20.8                                      |                                            |                                                     |                                                       |
| Ethanedioyl dichloride   | lq             | -367.6                                     |                                            |                                                     |                                                       |
| 1,2-Ethanedithiol        | lq             | -54.4                                      |                                            |                                                     |                                                       |
| Ethanethiol              | lq             | -73.6                                      | -5.5                                       | 207.0                                               | 117.9                                                 |
|                          | g              | -46.1                                      | -4.8                                       | 296.1                                               | 72.7                                                  |
| Ethanol                  | lq             | -277.6                                     | -174.8                                     | 161.0                                               | 112.3                                                 |
|                          | g              | -234.8                                     | -167.9                                     | 281.6                                               | 65.6                                                  |
| Ethene (see Ethylene)    |                |                                            |                                            |                                                     |                                                       |
| Ethoxybenzene            | lq             | -152.6                                     |                                            |                                                     | 228.5                                                 |
| 2-Ethoxyethyl acetate    | lq             |                                            |                                            |                                                     | 376.0                                                 |
| 2-Ethoxyethanol          | lq             |                                            |                                            |                                                     | 210.8                                                 |
| Ethyl acetate            | lq             | -479.3                                     | -332.7                                     | 257.7                                               | 170.7                                                 |
|                          | g              | -443.6                                     | -327.4                                     | 362.8                                               | 113.6                                                 |
| Ethylamine               | lq             |                                            |                                            |                                                     | 130.0                                                 |
|                          | g              | -47.4                                      | 36.3                                       | 283.8                                               | 71.5                                                  |
| Ethyl 4-aminobenzoate    | c              | -418.0                                     |                                            |                                                     |                                                       |
| N-Ethylaniline           | lq             | 4.0                                        | 188.7                                      | 239.3                                               |                                                       |
| Ethylbenzene             | lq             | -12.3                                      |                                            |                                                     | 183.2                                                 |
|                          | g              | 29.9                                       | 130.6                                      | 360.5                                               |                                                       |
| Ethyl benzoate           | lq             |                                            |                                            |                                                     | 246.0                                                 |
| 2-Ethylbenzoic acid      | c              | -441.3                                     |                                            |                                                     |                                                       |
| 3-Ethylbenzoic acid      | c              | -445.8                                     |                                            |                                                     |                                                       |
| 4-Ethylbenzoic acid      | c              | -460.7                                     |                                            |                                                     |                                                       |
| 2-Ethyl-1-butene         | g              | -56.0                                      | 80.0                                       | 376.6                                               | 133.6                                                 |
| Ethyl trans-2-butenolate | lq             | -420.1                                     |                                            |                                                     | 228.0                                                 |
| (ethyl crotonate)        |                |                                            |                                            |                                                     |                                                       |
| Ethyl carbamate          | c              | -520.5                                     |                                            |                                                     |                                                       |
| Ethyl 4-chlorobutanoate  | lq             | -566.5                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                            | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Ethyl chloroformate                  | lq             | -505.1                                     |                                            |                                                     |                                                       |
| Ethylcyclobutane                     | g              | -27.5                                      |                                            |                                                     |                                                       |
| Ethylcyclohexane                     | lq             | -211.9                                     | 29.1                                       | 280.9                                               | 211.8                                                 |
|                                      | g              | -171.7                                     | 39.3                                       | 382.6                                               | 158.8                                                 |
| 1-Ethylcyclohexene                   | lq             | -106.7                                     |                                            |                                                     |                                                       |
| Ethylcyclopentane                    | lq             | -163.4                                     | 37.3                                       | 279.9                                               | 185.8                                                 |
| 1-Ethylcyclopentene                  | g              | -19.7                                      |                                            |                                                     |                                                       |
| Ethylcyclopropane                    | lq             | -24.8                                      |                                            |                                                     |                                                       |
| Ethyl diethylcarbamate               | lq             | -592.3                                     |                                            |                                                     |                                                       |
| Ethyl 2,2-dimethylpropanoate         | lq             | -577.2                                     |                                            |                                                     |                                                       |
|                                      | g              | -536.0                                     |                                            |                                                     |                                                       |
| Ethylene                             | g              | 52.5                                       | 68.4                                       | 219.3                                               | 42.9                                                  |
| Ethylene- <i>d</i> <sub>4</sub>      | g              | 38.2                                       | 59.2                                       | 230.5                                               | 51.9                                                  |
| Ethylene carbonate                   | c              | -581.5                                     |                                            |                                                     | 133.9                                                 |
| Ethylenediaminetetra-<br>acetic acid | c              | -1759.4                                    |                                            |                                                     |                                                       |
| Ethylenediammonium chloride          | c              | -513.4                                     |                                            |                                                     |                                                       |
| 2,2'-(Ethylenedioxy)bis-<br>ethanol  | lq             | -804.2                                     |                                            |                                                     |                                                       |
| Ethylene glycol dibutyl ether        | lq             |                                            |                                            |                                                     | 350 <sup>20</sup>                                     |
| Ethylene glycol diethyl ether        | lq             | -451.4                                     |                                            |                                                     | 259.4                                                 |
| Ethylene glycol dimethyl ether       | lq             | -376.6                                     |                                            |                                                     | 193.3                                                 |
| Ethyleneimine                        | lq             | 91.9                                       |                                            |                                                     |                                                       |
|                                      | g              | 126.5(9)                                   | 178.0                                      | 250.6                                               | 52.6                                                  |
| Ethylene oxide                       | lq             | -78.0                                      | -11.8                                      | 153.9                                               | 88.0                                                  |
|                                      | g              | -52.6(6)                                   | -13.1                                      | 242.4                                               | 47.9                                                  |
| Ethyl formate                        | lq             |                                            |                                            |                                                     | 149.3                                                 |
| 2-Ethylhexanal                       | lq             | -342.5                                     |                                            |                                                     |                                                       |
| 3-Ethylhexane                        | lq             | -250.4                                     |                                            |                                                     |                                                       |
|                                      | g              | -210.7                                     |                                            |                                                     |                                                       |
| 2-Ethyl-1-hexanol                    | lq             | -432.8                                     |                                            | 347.0                                               | 317.5                                                 |
| Ethyl hydroperoxide                  | g              | 198.9                                      |                                            |                                                     |                                                       |
| Ethylidenecyclohexane                | lq             | -103.5                                     |                                            |                                                     |                                                       |
| Ethylidenecyclopentane               | lq             | -56.7                                      |                                            |                                                     |                                                       |
| Ethyl isocyanide                     | lq             | 108.4                                      |                                            |                                                     |                                                       |
| Ethyl isopropyl sulfide              | lq             | -156.1                                     |                                            |                                                     |                                                       |
| Ethyl lactate                        | lq             |                                            |                                            |                                                     | 254                                                   |
| Ethyllithium                         | c              | -58.6                                      |                                            |                                                     |                                                       |
| Ethylmercury bromide                 | c              | -107.5                                     |                                            |                                                     |                                                       |
| Ethylmercury chloride                | c              | -141.1                                     |                                            |                                                     |                                                       |
| Ethylmercury iodide                  | c              | -65.7                                      |                                            |                                                     |                                                       |
| 1-Ethyl-2-methylbenzene              | g              | 1.3                                        | 131.1                                      | 399.2                                               | 157.9                                                 |
| 2-Ethyl-3-methyl-1-butene            | g              | -79.5                                      |                                            |                                                     |                                                       |
| Ethyl 2-methylbutanoate              | lq             | -566.8                                     |                                            |                                                     |                                                       |
| Ethyl 3-methylbutanoate              | lq             | -570.9                                     |                                            |                                                     |                                                       |
| Ethyl methyl ether                   | g              | -216.4                                     | -117.7                                     | 309.2                                               | 93.3                                                  |
| 3-Ethyl-2-methylpentane              | lq             | -249.6                                     |                                            |                                                     |                                                       |
|                                      | g              | -211.0                                     | 21.3                                       | 441.1                                               |                                                       |
| 3-Ethyl-3-methylpentane              | lq             | -252.8                                     |                                            |                                                     |                                                       |
|                                      | g              | -214.8                                     | 19.9                                       | 433.0                                               |                                                       |
| 3-Ethyl-2-methyl-1-pentene           | g              | -100.3                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                    | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Ethyl methyl sulfide         | lq             | -91.6                                      |                                            | 239.1                                               | 144.6                                                 |
|                              | g              | -59.6                                      | 11.4                                       | 333.1                                               | 95.1                                                  |
| Ethyl nitrate                | g              | -154.1                                     | -36.9                                      | 348.3                                               | 97.4                                                  |
| Ethyl nitrite                | g              | -104.2                                     |                                            | 103.5                                               | 99.2                                                  |
| 1-Ethyl-2-nitrobenzene       | lq             | -48.7                                      |                                            |                                                     |                                                       |
| 1-Ethyl-4-nitrobenzene       | lq             | -55.4                                      |                                            |                                                     |                                                       |
| Ethyl 3-oxobutanoate         | lq             |                                            |                                            |                                                     | 248.0                                                 |
| 3-Ethylpentane               | lq             | -224.9                                     |                                            | 314.5                                               | 219.6                                                 |
|                              | g              | -189.6                                     | 11.0                                       | 411.5                                               | 166.0                                                 |
| Ethyl pentanoate             | lq             | -553.0                                     |                                            |                                                     |                                                       |
| 2-Ethylphenol                | lq             |                                            | -208.8                                     |                                                     |                                                       |
| 3-Ethylphenol                | lq             | -214.3                                     |                                            |                                                     |                                                       |
| 4-Ethylphenol                | c              | -224.4                                     |                                            |                                                     | 206.9                                                 |
| Ethylphosphonic acid         | c              | -1051.4                                    |                                            |                                                     |                                                       |
| Ethylphosphonic dichloride   | lq             | -613.4                                     |                                            |                                                     |                                                       |
| Ethyl propanoate             | lq             | -502.7                                     |                                            |                                                     | 196.1                                                 |
|                              | g              | -463.3                                     | -323.7                                     |                                                     |                                                       |
| Ethyl propyl ether           | g              | -272.2                                     |                                            | 295.0                                               | 197.2                                                 |
| Ethyl propyl sulfide         | lq             | -144.8                                     |                                            | 309.5                                               | 198.4                                                 |
|                              | g              | -104.7                                     | 23.6                                       | 414.1                                               | 139.3                                                 |
| 2-Ethylpyridine              | lq             | 7.4                                        |                                            |                                                     |                                                       |
| S-Ethyl thioacetate          | lq             | -268.2                                     |                                            |                                                     |                                                       |
| 2-Ethyltoluene               | g              | 1.3                                        | 131.1                                      | 399.2                                               | 157.9                                                 |
| 3-Ethyltoluene               | g              | -1.8                                       | 126.4                                      | 404.2                                               | 152.2                                                 |
| 4-Ethyltoluene               | g              | -3.2                                       | 85.3                                       | 398.9                                               | 151.5                                                 |
| N-Ethylurea                  | c              | -357.8                                     |                                            |                                                     |                                                       |
| Ethyl $\beta$ -vinylacrylate | lq             | -338.1                                     |                                            |                                                     |                                                       |
| Ethyl vinyl ether            | lq             | -167.4                                     |                                            |                                                     |                                                       |
|                              | g              | -140.8                                     |                                            |                                                     |                                                       |
| Ethynylbenzene               | g              | 327.3                                      | 361.8                                      | 321.7                                               | 114.9                                                 |
| Ethynylsilane                | g              |                                            |                                            | 269.4                                               | 72.6                                                  |
| Fluoranthene                 | c              | 189.9                                      | 345.6                                      | 230.5                                               | 230.2                                                 |
| Fluoroacetamide              | c              | -496.6                                     |                                            |                                                     |                                                       |
| Fluoroacetic acid            | c              | -688.3                                     |                                            |                                                     |                                                       |
| Fluoroacetylene              | g              |                                            |                                            | 269.4                                               | 72.6                                                  |
| Fluorobenzene                | lq             | -150.6                                     |                                            | 205.9                                               | 146.4                                                 |
|                              | g              | -116.0                                     | -69.0                                      | 302.6                                               | 94.4                                                  |
| 2-Fluorobenzoic acid         | c              | -567.6                                     |                                            |                                                     |                                                       |
| 3-Fluorobenzoic acid         | c              | -582.0                                     |                                            |                                                     |                                                       |
| 4-Fluorobenzoic acid         | c              | -585.7                                     |                                            |                                                     |                                                       |
| Fluoroethane                 | g              | -263.2                                     | -211.0                                     | 264.5                                               | 58.6                                                  |
| 2-Fluoroethanol              | lq             | -465.7                                     |                                            |                                                     |                                                       |
| Fluoroethylene               | g              | -138.8                                     |                                            |                                                     |                                                       |
| Fluoromethane                | g              | -237.8                                     | -213.8                                     | 222.8                                               | 37.5                                                  |
| 1-Fluoropropane              | g              | -285.9                                     | -200.3                                     | 304.2                                               | 82.6                                                  |
| 2-Fluoropropane              | g              | -293.5                                     | -204.2                                     | 292.1                                               | 82.0                                                  |
| Fluorosyltrifluoromethane    | g              | -766.0                                     | -707.0                                     | 322.4                                               | 79.4                                                  |
| 4-Fluorotoluene              | lq             | -186.9                                     | -79.8                                      | 237.1                                               | 171.2                                                 |
| Fluorotribromomethane        | g              | -190.4                                     | -193.1                                     | 345.8                                               |                                                       |
| Fluorotrinitromethane        | lq             | -220.9                                     |                                            |                                                     |                                                       |
| Formaldehyde                 | g              | -108.6                                     | -102.5                                     | 218.8                                               | 35.4                                                  |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                                     | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|---------------------------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Formamide                                                     | lq             | -254.0                                     |                                            |                                                     | 107.6                                                 |
|                                                               | g              | -193.9                                     | -141.0                                     | 248.6                                               | 45.4                                                  |
| Formanilide                                                   | c              | -151.5                                     |                                            |                                                     |                                                       |
| Formic acid                                                   | lq             | -424.7                                     | -361.4                                     | 129.0                                               | 99.5                                                  |
|                                                               | g              | -378.7                                     | -351.0                                     | 248.7                                               | 45.2                                                  |
| Formyl fluoride                                               | g              | -376.6                                     | -368.1                                     | 246.5(8)                                            | 40.0                                                  |
| D-(-)-Fructose                                                | c              | -1265.6                                    |                                            |                                                     |                                                       |
| D-(+)-Fucose                                                  | c              | -1099.1                                    |                                            |                                                     |                                                       |
| Fullerene-C <sub>60</sub>                                     | c              | 2327.0                                     | 2302.0                                     | 426.0                                               | 520.0                                                 |
| Fumaric acid                                                  | c              | -811.7                                     | -655.6                                     | 168.0                                               | 142.0                                                 |
| Fumaronitrile                                                 | c              | 268.2                                      |                                            |                                                     |                                                       |
| Furan                                                         | lq             | -62.3                                      |                                            | 177.0                                               | 114.8                                                 |
|                                                               | g              | -34.9                                      | 0.88                                       | 267.2                                               | 65.4                                                  |
| 2-Furancarboxaldehyde                                         | lq             | -201.6                                     |                                            |                                                     | 163.2                                                 |
| 2-Furancarboxylic acid                                        | c              | -498.4                                     |                                            |                                                     |                                                       |
| 2-Furanmethanol                                               | lq             | -276.2                                     | -154.2                                     | 215.5                                               | 204.0                                                 |
| Furfuryl alcohol                                              | lq             | -276.2                                     |                                            |                                                     | 204.0                                                 |
| Furylacrylic acid                                             | c              | -459.0                                     |                                            |                                                     |                                                       |
| Furylethylene                                                 | lq             | -10.5                                      |                                            |                                                     |                                                       |
| D-(+)-Galactose                                               | c              | -1286.3                                    | -918.8                                     | 205.4                                               |                                                       |
| D-Gluconic acid                                               | c              | -1587.0                                    |                                            |                                                     |                                                       |
| D-(+)-Glucose                                                 | c              | -1273.3                                    | -910.4                                     | 212.1                                               |                                                       |
| D-(-)-Glutamic acid                                           | c              | -1009.7                                    | -727.5                                     | 191.2                                               |                                                       |
| L-(+)-Glutamic acid                                           | c              | -1005.2                                    | -731.3                                     | 188.2                                               |                                                       |
| L-Glutamine                                                   | c              | -826.4                                     |                                            |                                                     |                                                       |
| Glutaric acid                                                 | c              | -960.0                                     |                                            |                                                     |                                                       |
| Glyceraldehyde                                                | lq             | -598.0                                     |                                            |                                                     |                                                       |
| Glycerol                                                      | lq             | -668.5                                     | -477.0                                     | 206.3                                               | 218.9                                                 |
| Glyceryl 1-acetate                                            | lq             | -909.1                                     |                                            |                                                     |                                                       |
| Glyceryl 1-benzoate                                           | c              | -777.3                                     |                                            |                                                     |                                                       |
| Glyceryl 2-benzoate                                           | c              | -772.8                                     |                                            |                                                     |                                                       |
| Glyceryl 1,3-diacetate                                        | lq             | -1120.7                                    |                                            |                                                     |                                                       |
| Glyceryl 1-dodecanoate                                        | c              | -1160.9                                    |                                            |                                                     |                                                       |
| Glyceryl 2-dodecanoate                                        | c              | -1152.6                                    |                                            |                                                     |                                                       |
| Glyceryl 1-hexadecanoate                                      | c              | -1281.5                                    |                                            |                                                     |                                                       |
| Glyceryl 1-hexanoate                                          | c              | -1109.0                                    |                                            |                                                     |                                                       |
| Glyceryl 2-hexanoate                                          | c              | -1095.8                                    |                                            |                                                     |                                                       |
| Glyceryl 1-octadecanoate                                      | c              | -1324.8                                    |                                            |                                                     |                                                       |
| Glyceryl 1-tetradecanoate                                     | c              | -1222.6                                    |                                            |                                                     |                                                       |
| Glyceryl triacetate                                           | lq             | -1330.8                                    |                                            |                                                     |                                                       |
| Glyceryl trinitrate                                           | lq             | -370.9                                     |                                            |                                                     |                                                       |
| Glyceryl tris(dodecanoate)                                    | c              | -2046.0                                    |                                            |                                                     |                                                       |
| Glyceryl tris(tetradecanoate)                                 | c              | -2176.0                                    |                                            |                                                     |                                                       |
| Glycine                                                       | c              | -528.5                                     | -368.6                                     | 103.5                                               | 99.2                                                  |
| ionized; std. state                                           | aq             | -469.8                                     | -315.0                                     | 111.0                                               |                                                       |
| <sup>+</sup> H <sub>3</sub> NCH <sub>2</sub> COOH; std. state | aq             | -517.9                                     | -384.2                                     | 190.2                                               |                                                       |
| Glycylglycine                                                 | c              | -747.7                                     | -490.6                                     | 190.0                                               |                                                       |
| Glyoxal                                                       | g              | -212.0                                     |                                            |                                                     |                                                       |
| Glyoxime                                                      | c              | -90.5                                      |                                            |                                                     |                                                       |
| Glyoxylic acid                                                | c              | -835.5                                     |                                            |                                                     |                                                       |
| Guanidine                                                     | c              | -56.0                                      |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                      | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Guanidine carbonate            | c              | -971.9                                     | -557.4                                     | 295.4                                               | 258.9                                                 |
| Guanidine nitrate              | c              | -387.0                                     |                                            |                                                     |                                                       |
| Guanidine sulfate              | c              | -1205.0                                    |                                            |                                                     |                                                       |
| Guanine                        | c              | -183.9                                     | 47.4                                       | 160.3                                               |                                                       |
| Guanylurea nitrate             | c              | -427.2                                     |                                            |                                                     |                                                       |
| L-Gulonic acid-γ-lactone       | c              | -1219.6                                    |                                            |                                                     |                                                       |
| Heptadecane                    | g              | -393.9                                     | 82.1                                       | 817.3                                               | 394.7                                                 |
| Heptadecanoic acid             | c              | -924.4                                     |                                            |                                                     | 475.7                                                 |
| 1-Heptadecene                  | g              | -268.4                                     | 179.9                                      | 813.1                                               | 383.9                                                 |
| Heptanal                       | lq             | -311.5                                     | -100.6                                     | 335.4                                               | 230.1                                                 |
|                                | g              | -264.0                                     | -86.7                                      | 461.7                                               |                                                       |
| Heptane                        | lq             | -224.2                                     |                                            |                                                     | 224.9                                                 |
|                                | g              | -187.7                                     | 8.0                                        | 427.9                                               | 166.0                                                 |
| Heptanedioic acid              | c              | -1009.4                                    |                                            |                                                     |                                                       |
| Heptanenitrile                 | lq             | -82.8                                      |                                            |                                                     |                                                       |
| 1-Heptanethiol                 | g              | -150.0                                     | 36.2                                       | 493.3                                               | 186.9                                                 |
| Heptanoic acid                 | lq             | -610.2                                     |                                            |                                                     | 265.4                                                 |
| 1-Heptanol                     | lq             | -403.3                                     | -142.3                                     | 320.1                                               | 272.1                                                 |
|                                | g              | -336.4                                     | -120.9                                     | 480.3                                               | 178.7                                                 |
| 2-Heptanone                    | lq             |                                            |                                            |                                                     | 232.6                                                 |
| 1-Heptene                      | lq             | -97.9                                      |                                            | 327.6                                               | 211.8                                                 |
|                                | g              | -62.3                                      | 95.8                                       | 423.6                                               | 155.2                                                 |
| cis-2-Heptene                  | lq             | -105.1                                     |                                            |                                                     |                                                       |
| trans-2-Heptene                | lq             | -109.5                                     |                                            |                                                     |                                                       |
| cis-3-Heptene                  | lq             | -104.3                                     |                                            |                                                     |                                                       |
| trans-3-Heptene                | lq             | -109.3                                     |                                            |                                                     |                                                       |
| 1-Heptyne                      | g              | 103.0                                      | 226.7                                      | 407.7                                               | 151.1                                                 |
| Hexabromoethane                | g              |                                            |                                            | 441.9                                               | 139.3                                                 |
| Hexachlorobenzene              | c              | -127.6                                     | 1.1                                        | 260.2                                               | 201.3                                                 |
|                                | g              | -35.5                                      | 44.2                                       | 441.2                                               | 173.2                                                 |
| Hexachloroethane               | c              | -202.8                                     |                                            | 237.3                                               | 198.2                                                 |
|                                | g              | -143.6                                     | -54.9                                      | 398.7                                               | 136.7                                                 |
| Hexadecafluoroethylcyclohexane | lq             | -3420.0                                    |                                            |                                                     |                                                       |
| Hexadecafluoroheptane          | lq             | -3420.8                                    | -3093.0                                    | 561.8                                               | 419.0                                                 |
| Hexadecane                     | lq             | -456.1                                     |                                            |                                                     | 501.6                                                 |
|                                | g              | -374.8                                     | 83.7                                       | 778.3                                               | 371.8                                                 |
| Hexadecanoic acid              | c              | -891.5                                     | -316.1                                     | 452.4                                               | 460.7                                                 |
| 1-Hexadecanol                  | c              | -686.7                                     | -98.7                                      | 451.9                                               | 422.0                                                 |
|                                | lq             | -635.4                                     | -96.6                                      | 606.7                                               |                                                       |
| 1-Hexadecene                   | lq             | -328.7                                     |                                            | 587.9                                               | 488.9                                                 |
|                                | g              | -248.5                                     | 171.5                                      | 774.1                                               | 361.0                                                 |
| 1,5-Hexadiene                  | lq             | 54.1                                       |                                            |                                                     |                                                       |
| 2,4-Hexadienoic acid           | c              | -390.8                                     |                                            |                                                     |                                                       |
| 1,5-Hexadiyne                  | lq             | 384.2                                      |                                            |                                                     |                                                       |
| Hexafluoroacetone              | g              | -1249.3                                    |                                            |                                                     |                                                       |
| Hexafluoroacetylacetone        | c              | -2286.7                                    |                                            |                                                     |                                                       |
| Hexafluorobenzene              | lq             | -991.3                                     |                                            | 280.8                                               | 156.6                                                 |
|                                | g              | -955.4                                     | -79.4                                      | 383.2                                               |                                                       |
| Hexafluoroethane               | g              | -1344.2                                    | -1255.8                                    | 332.3                                               | 106.7                                                 |
| cis-Hexahydroindane            | g              | -127.2                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                          | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| <i>trans</i> -Hexahydroindane      | g              | -131.4                                     |                                            |                                                     |                                                       |
| Hexamethylbenzene                  | c              | -162.4                                     | 117.4                                      | 306.3                                               | 245.6                                                 |
| 1,1,1,3,3,3-Hexamethyl-di-silazane | lq             | -518.0                                     |                                            |                                                     |                                                       |
| Hexamethyldisiloxane               | lq             | -814.6                                     | -541.8                                     | 433.8                                               | 311.4                                                 |
|                                    | g              | -777.7                                     | -534.5                                     | 535.0                                               | 238.5                                                 |
| Hexamethylenetetramine             | c              | 125.5                                      | 434.8                                      | 163.4                                               |                                                       |
| Hexamethylphosphoric triamide      | lq             |                                            |                                            |                                                     | 321                                                   |
| Hexanal                            | g              | -248.4                                     | -100.1                                     | 422.9                                               | 148.2                                                 |
| Hexanamide                         | c              | -423.0                                     |                                            |                                                     |                                                       |
|                                    | lq             | -397.0                                     |                                            |                                                     |                                                       |
| Hexane                             | lq             | -198.8                                     | -3.8                                       | 296.1                                               | 195.6                                                 |
|                                    | g              | -167.1(8)                                  | -0.25                                      | 388.4                                               | 143.1                                                 |
| 1,6-Hexanedioic acid               | lq             | -985.4                                     | -207.3                                     |                                                     | 232.2                                                 |
| 1,2-Hexanediol                     | lq             | -577.1                                     |                                            |                                                     |                                                       |
| 1,6-Hexanediol                     | c              | -569.9                                     |                                            |                                                     |                                                       |
| Hexanedinitrile                    | lq             | 85.1                                       |                                            |                                                     | 128.7                                                 |
| 1-Hexanethiol                      | g              | -129.9                                     | 27.8                                       | 454.3                                               | 164.1                                                 |
| Hexanoic acid                      | lq             | -583.9                                     |                                            |                                                     | 225.0                                                 |
| 1-Hexanol                          | lq             | -377.5                                     | -152.3                                     | 287.4                                               | 240.4                                                 |
|                                    | g              | -317.6                                     | -135.6                                     | 441.4                                               | 155.6                                                 |
| 2-Hexanol                          | lq             | -392.9                                     |                                            |                                                     |                                                       |
| 3-Hexanol                          | lq             | -392.4                                     |                                            |                                                     | 286.2                                                 |
| 2-Hexanone                         | lq             | -322.0                                     |                                            |                                                     | 213.3                                                 |
| 3-Hexanone                         | lq             | -320.2                                     |                                            | 305.3                                               | 216.9                                                 |
| 1-Hexene                           | lq             | -74.1                                      | 83.6                                       | 295.1                                               | 183.3                                                 |
|                                    | g              | -43.5                                      | 84.45                                      | 384.6                                               | 132.3                                                 |
| <i>cis</i> -2-Hexene               | lq             | -83.9                                      |                                            |                                                     |                                                       |
|                                    | g              | -52.3                                      | 76.2                                       | 386.5                                               | 125.7                                                 |
| <i>trans</i> -2-Hexene             | lq             | -85.5                                      |                                            |                                                     |                                                       |
|                                    | g              | -53.9                                      | 76.4                                       | 380.6                                               | 132.4                                                 |
| <i>cis</i> -3-Hexene               | lq             | -79.0                                      |                                            |                                                     |                                                       |
|                                    | g              | -47.6                                      | 83.0                                       | 379.6                                               | 123.6                                                 |
| <i>trans</i> -3-Hexene             | lq             | -86.1                                      |                                            |                                                     |                                                       |
| Hexyl acetate                      | lq             |                                            |                                            |                                                     | 282.8                                                 |
|                                    | g              | -54.4                                      | 77.6                                       | 374.8                                               | 132.8                                                 |
| 1-Hexyne                           | g              | 123.6                                      | 218.6                                      | 368.7                                               | 128.2                                                 |
| (-)-Histidine                      | c              | -466.7                                     |                                            |                                                     |                                                       |
| Hydantoin                          | c              | -448.5                                     |                                            |                                                     |                                                       |
| Hydrazine                          | lq             | 50.6                                       | 149.2                                      | 121.2                                               | 98.9                                                  |
| Hydrazinecarbothioamide            | c              | 24.7                                       |                                            |                                                     |                                                       |
| Hydrazobenzene                     | c              | 221.3                                      |                                            |                                                     |                                                       |
| Hydroxyacetic acid                 | c              | -663.6                                     |                                            |                                                     |                                                       |
| 2'-Hydroxyacetophenone             | c              | -357.7                                     |                                            |                                                     |                                                       |
| 3'-Hydroxyacetophenone             | c              | 370.7                                      |                                            |                                                     |                                                       |
| 4'-Hydroxyacetophenone             | c              | -364.4                                     |                                            |                                                     |                                                       |
| 2-Hydroxybenzaldehyde              | lq             | -279.9                                     |                                            |                                                     |                                                       |
| 2-Hydroxybenzaldoxime              | c              | -183.7                                     |                                            |                                                     |                                                       |
| 2-Hydroxybenzoic acid              | c              | -589.9                                     | -421.3                                     | 178.2                                               | 159.1                                                 |
| 3-Hydroxybenzoic acid              | c              | -584.9                                     | -417.3                                     | 177.0                                               | 157.3                                                 |
| 4-Hydroxybenzoic acid              | c              | -584.5                                     | -416.5                                     | 175.7                                               | 155.1                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                   | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|---------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| (±)-2-Hydroxybutanoic acid                  | lq             | − 679.1                                    |                                            |                                                     |                                                       |
| 2-Hydroxy-2,4,6-cyclohepta-<br>trienone     | c              | − 239.2                                    |                                            |                                                     |                                                       |
| 2-Hydroxyisobutanoic acid                   | c              | − 744.3                                    |                                            |                                                     |                                                       |
| 2-Hydroxy-1-isopropyl-4-<br>methylbenzene   | c              | − 309.6                                    |                                            |                                                     |                                                       |
| 3-Hydroxy-4-methoxybenz-<br>aldehyde        | c              | − 453.6                                    |                                            |                                                     |                                                       |
| 4-Hydroxy-4-methyl-2-<br>pentanone          | lq             |                                            |                                            |                                                     | 221.3                                                 |
| 2-Hydroxymethyl-1,3-propane-<br>diol        | c              | − 744.6                                    |                                            |                                                     |                                                       |
| 3-Hydroxy-2-naphthalene-<br>carboxylic acid | c              | − 547.7                                    |                                            |                                                     |                                                       |
| 5-Hydroxy-1-pentanal                        | lq             | − 479.9                                    |                                            |                                                     |                                                       |
| <i>trans</i> -(−)-4-Hydroxyproline          | c              | − 661.1                                    |                                            |                                                     |                                                       |
| ( <i>S</i> )-2-Hydroxypropanoic acid        | c              | − 694.0                                    |                                            |                                                     |                                                       |
| 2-Hydroxypropanonitrile                     | lq             | − 138.9                                    | 34.3                                       |                                                     |                                                       |
| 2-Hydroxypyridine                           | c              | − 166.3                                    |                                            |                                                     |                                                       |
| 3-Hydroxypyridine                           | c              | − 132.0                                    |                                            |                                                     |                                                       |
| 4-Hydroxypyridine                           | c              | − 144.6                                    |                                            |                                                     |                                                       |
| 8-Hydroxyquinoline                          | c              | − 81.2                                     |                                            |                                                     |                                                       |
| (−)-2-Hydroxysuccinic acid                  | c              | − 1103.7                                   | − 884.7                                    |                                                     |                                                       |
| (±)-2-Hydroxysuccinic acid                  | c              | − 1105.7                                   |                                            |                                                     |                                                       |
| Hypoxanthene                                | c              | − 110.8                                    | 76.9                                       | 145.6                                               | 134.5                                                 |
| Icosane                                     | g              | − 455.8                                    | 117.3                                      | 934.1                                               | 463.3                                                 |
| Icosanoic acid                              | c              | − 1011.9                                   |                                            |                                                     | 545.1                                                 |
| Icosene                                     | g              | − 330.2                                    | 205.1                                      | 929.9                                               | 452.5                                                 |
| Imidazole                                   | c              | 49.8                                       |                                            |                                                     |                                                       |
| Iminodiacetic acid                          | c              | − 932.6                                    |                                            |                                                     |                                                       |
| Indane                                      | lq             | 11.5                                       | 150.8                                      | 56.0                                                | 190.3                                                 |
| 1 <i>H</i> -Indazole                        | c              | 151.9                                      |                                            |                                                     |                                                       |
| Indene                                      | lq             | 110.6                                      | 217.6                                      | 215.3                                               | 186.9                                                 |
| 1 <i>H</i> -Indole                          | c              | 86.7                                       |                                            |                                                     |                                                       |
| Indole-2,3-dione                            | c              | − 268.2                                    |                                            |                                                     |                                                       |
| Iodoacetone                                 | g              | − 130.5                                    |                                            |                                                     |                                                       |
| Iodobenzene                                 | lq             | 117.1                                      |                                            | 205.4                                               | 158.7                                                 |
|                                             | g              | 164.9                                      | 187.8                                      | 334.1                                               | 100.8                                                 |
| 2-Iodobenzoic acid                          | c              | − 302.3                                    |                                            |                                                     |                                                       |
| 3-Iodobenzoic acid                          | c              | − 316.9                                    |                                            |                                                     |                                                       |
| 4-Iodobenzoic acid                          | c              | − 316.1                                    |                                            |                                                     |                                                       |
| Iodocyclohexane                             | lq             | − 97.2                                     |                                            |                                                     |                                                       |
| Iodoethane                                  | lq             | − 40.0                                     | 14.7                                       | 211.7                                               | 115.1                                                 |
|                                             | g              | − 8.1                                      | 19.2                                       | 306.0                                               | 66.9                                                  |
| Iodoethylene                                | g              |                                            |                                            | 285.0                                               | 57.9                                                  |
| Iodomethane                                 | g              | 14.4                                       | 15.6                                       | 254.1                                               | 44.1                                                  |
| 2-Iodo-2-methylpropane                      | lq             | − 107.5                                    |                                            |                                                     | 162.3                                                 |
|                                             | g              | − 72.0                                     | 23.6                                       | 342.2                                               | 118.3                                                 |
| 1-Iodonaphthalene                           | lq             | 161.5                                      |                                            |                                                     |                                                       |
| 2-Iodonaphthalene                           | c              | 144.3                                      |                                            |                                                     |                                                       |
| 2-Iodophenol                                | c              | − 95.8                                     |                                            |                                                     |                                                       |
| 3-Iodophenol                                | c              | − 94.5                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                   | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 4-Iodophenol                | c              | -95.4                                      |                                            |                                                     |                                                       |
| 1-Iodopropane               | lq             | -66.0                                      |                                            |                                                     | 126.8                                                 |
|                             | g              | -30.0                                      |                                            |                                                     |                                                       |
| 2-Iodopropane               | lq             | -74.8                                      |                                            |                                                     | 91.0                                                  |
|                             | g              | -40.3                                      | 20.1                                       | 324.5                                               | 90.1                                                  |
| 3-Iodopropanoic acid        | c              | -460.0                                     |                                            |                                                     |                                                       |
| 3-Iodo-1-propene            | g              | 91.5                                       |                                            |                                                     |                                                       |
| $\alpha$ -Iodotoluene       | lq             | 57.7                                       |                                            |                                                     |                                                       |
| 3-Iodotoluene               | lq             | 79.1                                       |                                            |                                                     |                                                       |
| 4-Iodotoluene               | lq             | 67.4                                       |                                            |                                                     |                                                       |
| Isobutanenitrile            | g              | 25.4                                       | 103.6                                      | 313.3                                               | 96.4                                                  |
| Isobutylamine               | lq             | -132.6                                     |                                            |                                                     | 183.2                                                 |
| Isobutylbenzene             | lq             | -69.8                                      |                                            |                                                     |                                                       |
| Isobutyl trichloroacetate   | lq             | -553.4                                     |                                            |                                                     |                                                       |
| Isocyanomethane             | g              | 163.5                                      | 165.7                                      | 246.9                                               | 52.9                                                  |
| (-)-Isoleucine              | c              | -637.9                                     | -347.2                                     | 208.0                                               | 188.3                                                 |
| ( $\pm$ )-Isoleucine        | c              | -635.3                                     |                                            |                                                     |                                                       |
| Isoxazole                   | g              | 78.6                                       |                                            |                                                     |                                                       |
| Isopropenyl acetate         | lq             | -386.4                                     |                                            |                                                     |                                                       |
| Isopropyl acetate           | lq             | -518.9                                     |                                            |                                                     | 199.4                                                 |
| Isopropylamine              | lq             | -112.3                                     |                                            | 218.3                                               | 163.8                                                 |
|                             | g              | -83.7                                      | 32.2                                       | 312.2                                               | 97.5                                                  |
| Isopropylbenzene            | lq             | -41.1                                      | 124.3                                      | 279.8                                               | 210.7                                                 |
|                             | g              | 4.0                                        | 137.0                                      | 388.6                                               | 151.7                                                 |
| 1-Isopropyl-2-methylbenzene | lq             | -73.3                                      |                                            |                                                     |                                                       |
| 1-Isopropyl-3-methylbenzene | lq             | -78.6                                      |                                            |                                                     |                                                       |
| 1-Isopropyl-4-methylbenzene | lq             | -78.0                                      | 119.1                                      | 306.6                                               |                                                       |
| Isopropyl methyl ether      | lq             | -278.8                                     |                                            | 253.8                                               | 161.9                                                 |
|                             | g              | -252.0                                     | -120.9                                     | 332.3                                               | 111.1                                                 |
| 2-Isopropyl-5-methylphenol  | c              | -309.7                                     |                                            |                                                     |                                                       |
| Isopropyl methyl sulfide    | lq             | -105.7                                     |                                            | 263.1                                               | 172.4                                                 |
|                             | g              | -90.5                                      | 13.4                                       | 359.3                                               | 117.2                                                 |
| Isopropyl nitrate           | g              | -191.0                                     | -40.7                                      | 373.2                                               | 120.7                                                 |
| 2-Isopropylphenol           | lq             | -233.7                                     |                                            |                                                     |                                                       |
| 3-Isopropylphenol           | lq             | -252.5                                     |                                            |                                                     |                                                       |
| 4-Isopropylphenol           | lq             | -265.9                                     |                                            |                                                     |                                                       |
| Isopropyl thioacetate       | lq             | -298.2                                     |                                            |                                                     |                                                       |
| Isopropyl trichloroacetate  | lq             | -536.0                                     |                                            |                                                     |                                                       |
| Isoquinoline                | c              | 144.5                                      |                                            |                                                     |                                                       |
|                             | lq             |                                            |                                            |                                                     | 196.8                                                 |
| Ketene                      | g              | -47.5                                      | -48.3                                      | 247.6                                               | 51.8                                                  |
| (+)-Lactic acid             | c              | -694.1                                     | -522.9                                     | 142.3                                               |                                                       |
| ( $\pm$ )-Lactic acid       | lq             | -674.5                                     | -518.2                                     | 192.1                                               |                                                       |
| $\beta$ -Lactose            | c              | -2236.7                                    | -1567.0                                    | 386.2                                               |                                                       |
| (+)-Leucine                 | c              | -637.3                                     | -347.2                                     | 208.0                                               |                                                       |
| (-)-Leucine                 | c              | -637.4                                     | -346.3                                     | 211.8                                               | 201.0                                                 |
| (+)-Limonene                | lq             | -54.5                                      |                                            |                                                     | 249.0                                                 |
| ( $\pm$ )-Lysine            | c              | -678.6                                     |                                            |                                                     |                                                       |
| Malic acid                  | c              | -789.4                                     | -625.1                                     | 160.8                                               | 137.0                                                 |
| Maleic anhydride            | c              | -469.8                                     |                                            |                                                     |                                                       |
| (R)-Malic acid              | c              | -1105.7                                    |                                            |                                                     |                                                       |
| (S)-Malic acid              | c              | -1103.6                                    |                                            |                                                     |                                                       |



**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                       | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|---------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Malonamide                      | c              | − 546.0                                    |                                            |                                                     |                                                       |
| Malonic acid                    | c              | − 891.0                                    |                                            |                                                     |                                                       |
| Malonodiamide                   | c              | − 546.1                                    |                                            |                                                     |                                                       |
| Malononitrile                   | c              | 186.6                                      |                                            |                                                     |                                                       |
| D-(+)-Maltose                   | c              | − 2220.9                                   | − 1726.3                                   |                                                     |                                                       |
| (±)-Mandelic acid               | c              | − 579.4                                    |                                            |                                                     |                                                       |
| (+)-Mannitol                    | c              | − 1337.1                                   | − 942.2                                    | 238.5                                               |                                                       |
| D-(+)-Mannose                   | c              | − 1263.0                                   |                                            |                                                     |                                                       |
| 2-Mercaptopropanoic acid        | lq             | − 468.2                                    | − 343.9                                    | 228.9                                               |                                                       |
| Methane                         | g              | − 74.6                                     | − 50.5                                     | 186.3                                               | 35.7                                                  |
| Methane- <i>d</i> <sub>4</sub>  | g              | − 88.2                                     | − 59.5                                     | 198.9                                               | 40.3                                                  |
| Methanethiol                    | lq             | − 46.7                                     | − 7.7                                      | 169.2                                               | 90.5                                                  |
|                                 | g              | − 22.9                                     | − 9.9                                      | 255.1                                               | 50.3                                                  |
| Methanol                        | lq             | − 239.1                                    | − 166.6                                    | 126.8                                               | 81.2                                                  |
|                                 | g              | − 201.0                                    | − 162.3                                    | 239.9                                               | 44.1                                                  |
| (−)-Methionine                  | c              | − 577.5                                    | − 505.8                                    | 231.5                                               |                                                       |
| 2-Methoxybenzaldehyde           | c              | − 266.5                                    |                                            |                                                     |                                                       |
| 3-Methoxybenzaldehyde           | lq             | − 276.1                                    |                                            |                                                     |                                                       |
| 4-Methoxybenzaldehyde           | lq             | − 267.2                                    |                                            |                                                     |                                                       |
| Methoxybenzene                  | lq             | − 114.8                                    |                                            |                                                     | 199.0                                                 |
|                                 | g              | − 67.9                                     |                                            |                                                     |                                                       |
| 2-Methoxybenzoic acid           | c              | − 538.5                                    |                                            |                                                     |                                                       |
| 3-Methoxybenzoic acid           | c              | − 553.5                                    |                                            |                                                     |                                                       |
| 4-Methoxybenzoic acid           | c              | − 561.7                                    |                                            |                                                     |                                                       |
| 2-Methoxyethanol                | lq             |                                            |                                            |                                                     | 171.1                                                 |
| 2-Methoxyethyl acetate          | lq             |                                            |                                            |                                                     | 310.0                                                 |
| 2-Methoxytetrahydropyran        | lq             | − 442.3                                    |                                            |                                                     |                                                       |
| 5-Methoxytetrazole              | c              | 69.1                                       |                                            |                                                     |                                                       |
| 1-Methoxy-2,4,6-trinitrobenzene | c              | − 157.5                                    |                                            |                                                     |                                                       |
| Methyl (CH <sub>3</sub> )       | g              | 145.7                                      | 147.9                                      | 194.2                                               | 38.7                                                  |
| Methyl acetate                  | lq             | − 445.8                                    |                                            |                                                     | 141.9                                                 |
|                                 | g              | − 413.3                                    |                                            | 324.4                                               | 86.0                                                  |
| Methyl acrylate                 | lq             | − 362.2                                    | − 243.2                                    | 239.5                                               | 158.8                                                 |
|                                 | g              | − 333.0                                    | − 237.6                                    |                                                     |                                                       |
| Methylamine                     | lq             | − 47.2                                     | 35.7                                       | 150.2                                               | 102.1                                                 |
|                                 | g              | − 22.5                                     | 32.7                                       | 242.9                                               | 50.1                                                  |
| <i>N</i> -Methylaniline         | lq             | 32.2                                       |                                            |                                                     | 207.1                                                 |
| <i>o</i> -Methylaniline         | lq             | − 6.3                                      |                                            |                                                     | 209.6                                                 |
|                                 | g              | 56.4                                       | 167.6                                      | 351.0                                               | 130.2                                                 |
| <i>m</i> -Methylaniline         | lq             | − 8.1                                      |                                            |                                                     | 227.0                                                 |
|                                 | g              | 54.6                                       | 165.4                                      | 352.5                                               | 125.5                                                 |
| <i>p</i> -Methylaniline         | lq             | − 23.5                                     |                                            |                                                     |                                                       |
|                                 | g              | 55.3                                       | 167.7                                      | 347.0                                               | 126.2                                                 |
| Methyl benzoate                 | lq             | − 343.5                                    |                                            |                                                     | 221.3                                                 |
| 2-Methylbenzoic acid            | c              | − 416.5                                    |                                            |                                                     |                                                       |
|                                 | lq             |                                            |                                            |                                                     | 174.9                                                 |
| 3-Methylbenzoic acid            | c              | − 426.1                                    |                                            |                                                     |                                                       |
|                                 | lq             |                                            |                                            |                                                     | 163.6                                                 |
| 4-Methylbenzoic acid            | c              | − 429.2                                    |                                            |                                                     |                                                       |
|                                 | lq             |                                            |                                            |                                                     | 169.0                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                                    | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 2-Methylbenzoic anhydride                                    | c              | -533.5                                     |                                            |                                                     |                                                       |
| 4-Methylbenzoic anhydride                                    | c              | -520.9                                     |                                            |                                                     |                                                       |
| 1-Methylbicyclo[4.1.0]heptane                                | lq             | -59.9                                      |                                            |                                                     |                                                       |
| 1-Methylbicyclo[3.1.0]hexane                                 | lq             | -33.2                                      |                                            |                                                     |                                                       |
| 2-Methylbiphenyl                                             | lq             | 108.0                                      |                                            |                                                     |                                                       |
| 3-Methylbiphenyl                                             | lq             | 85.4                                       |                                            |                                                     |                                                       |
| 4-Methylbiphenyl                                             | c              | 55.2                                       |                                            |                                                     |                                                       |
| 2-Methyl-1,3-butadiene                                       | lq             | 48.2                                       |                                            | 229.3                                               | 152.6                                                 |
|                                                              | g              | 75.5                                       | 145.9                                      | 315.6                                               | 104.6                                                 |
| 3-Methyl-1,2-butadiene                                       | g              | 129.7                                      | 198.6                                      | 319.7                                               | 105.4                                                 |
| 2-Methylbutane                                               | lq             | -178.4                                     |                                            | 260.4                                               | 164.8                                                 |
|                                                              | g              | -154.0                                     | -14.8                                      | 343.6                                               | 118.8                                                 |
| 2-Methyl-2-butanethiol                                       | lq             | -162.8                                     |                                            | 290.1                                               | 198.1                                                 |
|                                                              | g              | -127.1                                     | 9.2                                        | 386.9                                               | 143.5                                                 |
| 3-Methyl-1-butanethiol                                       | g              | -114.9                                     |                                            |                                                     |                                                       |
| 3-Methyl-2-butanethiol                                       | lq             | -158.8                                     |                                            |                                                     |                                                       |
| 2-Methylbutanoic acid                                        | lq             | -554.4                                     |                                            |                                                     |                                                       |
| 3-Methylbutanoic acid                                        | lq             | -561.6                                     |                                            |                                                     | 197.1                                                 |
| 2-Methyl-1-butanol                                           | lq             | -356.6                                     |                                            |                                                     | 220.1                                                 |
| 3-Methyl-1-butanol                                           | lq             | -356.4                                     |                                            |                                                     | 210.0                                                 |
| 2-Methyl-2-butanol                                           | lq             | -379.5                                     | -175.3                                     | 229.3                                               | 247.1                                                 |
| (±)-3-Methyl-2-butanol                                       | lq             | -366.6                                     |                                            |                                                     | 232.2                                                 |
| 3-Methyl-2-butanone                                          | lq             | -299.5                                     |                                            | 268.5                                               | 179.9                                                 |
|                                                              | g              | -262.5                                     |                                            |                                                     |                                                       |
| 2-Methyl-1-butene                                            | lq             | -61.1                                      |                                            | 254.0                                               | 157.2                                                 |
|                                                              | g              | -35.3                                      | 65.6                                       | 339.5                                               | 110.0                                                 |
| 3-Methyl-1-butene                                            | lq             | -51.5                                      |                                            | 253.3                                               | 156.1                                                 |
|                                                              | g              | -27.6                                      | 74.8                                       | 333.5                                               | 118.6                                                 |
| 2-Methyl-2-butene                                            | lq             | -68.6                                      |                                            | 251.0                                               | 152.8                                                 |
|                                                              | g              | -41.8                                      | 59.7                                       | 338.6                                               | 105.0                                                 |
| <i>trans</i> -2-Methyl-2-butenedioic acid [also <i>cis</i> ] | c              | -824.4                                     |                                            |                                                     |                                                       |
| <i>cis</i> -2-Methyl-2-butenioic acid                        | c              | -455.6                                     |                                            |                                                     |                                                       |
| <i>trans</i> -2-Methyl-2-butenioic acid                      | c              | -490.8                                     |                                            |                                                     |                                                       |
| 3-Methylbutyl acetate                                        | lq             |                                            |                                            |                                                     | 248.5                                                 |
| 3-Methyl-1-butyne                                            | g              | 136.4                                      | 205.5                                      | 319.0                                               | 104.7                                                 |
| Methyl <i>trans</i> -2-butenioate                            | lq             | -382.8                                     |                                            |                                                     |                                                       |
| Methylcyclobutane                                            | lq             | -44.5                                      |                                            |                                                     |                                                       |
| Methylcyclobutanecarboxylic acid                             | lq             | -395.0                                     |                                            |                                                     |                                                       |
| Methylcyclohexane                                            | lq             | -190.1                                     | 20.3                                       | 247.9                                               | 184.9                                                 |
|                                                              | g              | -154.7                                     | 27.3                                       | 343.3                                               | 135.0                                                 |
| <i>cis</i> -2-Methylcyclohexanol                             | lq             | -390.2                                     |                                            |                                                     | 200 <sup>17</sup>                                     |
| <i>trans</i> -2-Methylcyclohexanol                           | lq             | -415.8                                     |                                            |                                                     | 200 <sup>17</sup>                                     |
| <i>cis</i> -3-Methylcyclohexanol                             | lq             | -416.1                                     |                                            |                                                     | 292 <sup>17</sup>                                     |
| <i>trans</i> -3-Methylcyclohexanol                           | lq             | -394.4                                     |                                            |                                                     | 202 <sup>17</sup>                                     |
| <i>cis</i> -4-Methylcyclohexanol                             | lq             | -413.2                                     |                                            |                                                     | 202 <sup>17</sup>                                     |
| <i>trans</i> -4-Methylcyclohexanol                           | lq             | -433.3                                     |                                            |                                                     | 202 <sup>17</sup>                                     |
| 2-Methylcyclohexene                                          | lq             | -81.2                                      |                                            |                                                     |                                                       |
| Methylcyclopentane                                           | lq             | -138.0                                     | 31.5                                       | 247.9                                               | 158.7                                                 |
|                                                              | g              | -106.2                                     | 35.8                                       | 339.9                                               | 109.8                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                     | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 1-Methylcyclopentanol         | lq             | − 343.3                                    |                                            |                                                     |                                                       |
| 2-Methylcyclopentanone        | lq             | − 265.3                                    |                                            |                                                     |                                                       |
| 1-Methylcyclopentene          | g              | − 3.8                                      | 102.1                                      | 326.4                                               | 100.8                                                 |
| 3-Methylcyclopentene          | g              | 7.4                                        | 115.0                                      | 330.5                                               | 100.0                                                 |
| 4-Methylcyclopentene          | g              | 14.6                                       | 121.6                                      | 328.9                                               | 100.0                                                 |
| 1-Methylcyclopropene          | lq             | 1.7                                        |                                            |                                                     |                                                       |
|                               | g              | 243.6                                      |                                            |                                                     |                                                       |
| Methylenecyclobutane          | g              | 121.6                                      |                                            |                                                     |                                                       |
| Methylenebutanedioic acid     | c              | − 841.1                                    |                                            |                                                     |                                                       |
| Methylenecyclohexane          | lq             | − 61.3                                     |                                            |                                                     |                                                       |
| Methylenecyclohexene          | lq             | − 12.7                                     |                                            |                                                     |                                                       |
| Methylenecyclopropane         | g              | 200.5                                      |                                            |                                                     |                                                       |
| Methyl decanoate              | lq             | − 640.4                                    |                                            |                                                     |                                                       |
| Methyl 2,2-dimethylpropanoate | lq             | − 530.0                                    |                                            |                                                     | 257.9                                                 |
| 2-Methyl-1,3-dioxane          | lq             | − 436.4                                    |                                            |                                                     |                                                       |
| 4-Methyl-1,3-dioxane          | c              | 416.1                                      |                                            |                                                     |                                                       |
| N-Methyldiphenylamine         | lq             | 120.5                                      |                                            |                                                     |                                                       |
| 4-Methyldiphenylamine         | c              | 49.0                                       |                                            |                                                     |                                                       |
| Methyl dodecanoate            | lq             | − 693.0                                    |                                            |                                                     |                                                       |
| Methylene (CH <sub>2</sub> )  | g              | 390.4                                      | 372.9                                      | 194.9                                               | 33.8                                                  |
| Methylenebutanedioic acid     | c              | − 841.1                                    |                                            |                                                     |                                                       |
| Methylenecyclohexane          | lq             | − 61.3                                     |                                            |                                                     |                                                       |
| 2-Methylenecyclohexanol       | lq             | − 277.6                                    |                                            |                                                     |                                                       |
| 3-Methylenecyclohexene        | lq             | − 12.7                                     |                                            |                                                     |                                                       |
| 2-Methylenecyclopentanol      | lq             | 46.9                                       |                                            |                                                     |                                                       |
| Methylenecyclopropane         | g              | 200.5                                      |                                            |                                                     |                                                       |
| Methylenesuccinic acid        | c              | − 841.2                                    |                                            |                                                     |                                                       |
| Methylene sulfate             | c              | − 688.7                                    |                                            |                                                     |                                                       |
| N-Methylformamide             | lq             |                                            |                                            |                                                     | 123.8                                                 |
| Methyl formate                | lq             | − 386.1                                    |                                            |                                                     | 119.1                                                 |
|                               | g              | − 357.4                                    | − 297.2                                    | 285.3                                               | 64.4                                                  |
| Methyl 2-furancarboxylate     | lq             | − 450.0                                    |                                            |                                                     |                                                       |
| 2-Methyl-2,5-furandione       | lq             | − 504.5                                    |                                            |                                                     |                                                       |
| α-Methyl-(+)-glucoside        | c              | − 1233.4                                   |                                            |                                                     |                                                       |
| N-Methylglycine               | c              | − 513.3                                    |                                            |                                                     |                                                       |
| Methylglyoxal                 | g              | − 27.1                                     |                                            |                                                     |                                                       |
| Methylglyoxime                | c              | − 126.8                                    |                                            |                                                     |                                                       |
| 2-Methylheptane               | lq             | − 255.0                                    |                                            | 356.4                                               | 252.0                                                 |
|                               | g              | − 215.4                                    | 12.8                                       | 452.5                                               |                                                       |
| 3-Methylheptane               | lq             | − 252.3                                    |                                            | 362.6                                               | 250.2                                                 |
|                               | g              | − 212.5                                    | 13.7                                       | 461.6                                               |                                                       |
| 4-Methylheptane               | lq             | − 251.6                                    |                                            |                                                     | 251.1                                                 |
|                               | g              | − 212.0                                    | 16.7                                       | 453.3                                               |                                                       |
| Methyl heptanoate             | lq             | − 567.1                                    |                                            |                                                     | 285.1                                                 |
| 2-Methylhexane                | lq             | − 229.5                                    |                                            | 323.3                                               | 222.9                                                 |
|                               | g              | − 194.6                                    | 3.2                                        | 420.0                                               | 166.0                                                 |
| 3-Methylhexane                | lq             | − 226.4                                    |                                            |                                                     | 214.2                                                 |
|                               | g              | − 192.3                                    | 4.6                                        | 424.1                                               | 166.0                                                 |
| Methyl hexanoate              | lq             | − 540.2                                    |                                            |                                                     |                                                       |
| 5-Methyl-1-hexene             | g              | − 65.7                                     |                                            |                                                     |                                                       |
| cis-3-Methyl-3-hexene         | g              | − 79.4                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                            | Physical State | $\Delta_f H^\circ$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $S^\circ$<br>$\text{J}\cdot\text{deg}^{-1}\cdot\text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J}\cdot\text{deg}^{-1}\cdot\text{mol}^{-1}$ |
|------------------------------------------------------|----------------|-------------------------------------------------------|-------------------------------------------------------|-----------------------------------------------------------------|-------------------------------------------------------------------|
| <i>trans</i> -3-Methyl-3-hexene                      | g              | −76.8                                                 |                                                       |                                                                 |                                                                   |
| Methylhydrazine                                      | lq             | 54.2                                                  | 179.9                                                 | 165.9                                                           | 134.9                                                             |
|                                                      | g              | 94.7                                                  | 186.9                                                 | 278.7                                                           | 71.1                                                              |
| 2-Methyl-1 <i>H</i> -indole                          | c              | 60.7                                                  |                                                       |                                                                 |                                                                   |
| 3-Methyl-1 <i>H</i> -indole                          | c              | 68.2                                                  |                                                       |                                                                 |                                                                   |
| Methyl isocyanate                                    | lq             | −92.0                                                 |                                                       |                                                                 |                                                                   |
| Methyl isocyanide                                    | g              | 163.5                                                 | 165.7                                                 | 246.8                                                           | 52.9                                                              |
| 1-Methyl-4-isopropylbenzene                          | lq             | −78.0                                                 |                                                       |                                                                 | 236.4                                                             |
| Methyl isopropyl sulfide                             | g              | −90.4                                                 | 13.4                                                  | 359.3                                                           | 117.2                                                             |
| Methyl isothiocyanate                                | c              | 79.4                                                  |                                                       |                                                                 |                                                                   |
|                                                      | g              | 131.0                                                 | 144.4                                                 | 252.3                                                           | 65.5                                                              |
| 5-Methylisoxazole                                    | lq             | −5.6                                                  |                                                       |                                                                 |                                                                   |
| Methylmercury bromide                                | c              | −86.2                                                 |                                                       |                                                                 |                                                                   |
| Methylmercury chloride                               | c              | −116.3                                                |                                                       |                                                                 |                                                                   |
| Methylmercury iodide                                 | c              | −43.5                                                 |                                                       |                                                                 |                                                                   |
| Methyl 2-methylbutanoate                             | lq             | −534.3                                                |                                                       |                                                                 |                                                                   |
| Methyl 3-methylbutanoate                             | lq             | −538.9                                                |                                                       |                                                                 |                                                                   |
| 7-Methyl-3-methylene-1,6-octadiene                   | lq             | 14.5                                                  |                                                       |                                                                 |                                                                   |
| ( <i>R</i> )-1-Methyl-4-(1-methylethenyl)cyclohexene | lq             | −54.5                                                 |                                                       |                                                                 | 249 <sup>20</sup>                                                 |
| 1-Methylnaphthalene                                  | lq             | 56.3                                                  | 189.4                                                 | 254.8                                                           | 224.4                                                             |
| 2-Methylnaphthalene                                  | c              | 44.9                                                  | 192.6                                                 | 220.0                                                           | 196.0                                                             |
|                                                      | g              | 106.7                                                 | 216.2                                                 | 380.0                                                           | 159.8                                                             |
| Methyl nitrate                                       | lq             | −156.3                                                | −43.5                                                 | 217.2                                                           | 157.3                                                             |
|                                                      | g              | −124.4                                                | −39.3                                                 | 318.5                                                           | 76.5                                                              |
| Methyl nitrite                                       | g              | −66.1                                                 | 1.0                                                   | 284.3                                                           | 63.2                                                              |
| Methyl nitroacetate                                  | lq             | −464.0                                                |                                                       |                                                                 |                                                                   |
| 2-Methyl-5-nitroaniline                              | c              | −91.3                                                 |                                                       |                                                                 |                                                                   |
| 4-Methyl-3-nitroaniline                              | c              | −71.7                                                 |                                                       |                                                                 |                                                                   |
| 1-Methyl-2-nitrobenzene                              | lq             | −9.7                                                  |                                                       |                                                                 |                                                                   |
| 1-Methyl-3-nitrobenzene                              | lq             | −31.5                                                 |                                                       |                                                                 |                                                                   |
| 1-Methyl-4-nitrobenzene                              | c              | −48.1                                                 |                                                       |                                                                 |                                                                   |
| 2-Methyl-2-nitropropane                              | c              | −229.8                                                |                                                       |                                                                 |                                                                   |
| 2-Methyl-2-nitro-1,3-propanediol                     | c              | −575.3                                                |                                                       |                                                                 |                                                                   |
| 2-Methyl-2-nitro-1-propanol                          | c              | −410.0                                                |                                                       |                                                                 |                                                                   |
| 2-Methylnonane                                       | lq             | −309.8                                                |                                                       | 420.1                                                           | 313.3                                                             |
| 5-Methylnonane                                       | lq             | −307.9                                                |                                                       | 423.8                                                           | 314.4                                                             |
| Methyl phenylcarbamate                               | c              | −186.7                                                |                                                       |                                                                 |                                                                   |
| Methyl <i>cis</i> -9-octadecanoate                   | lq             | −734.5                                                |                                                       |                                                                 |                                                                   |
| Methyl octanoate                                     | lq             | −590.3                                                |                                                       |                                                                 |                                                                   |
| 2-Methyl-2-oxazoline                                 | g              | −130.5                                                |                                                       |                                                                 |                                                                   |
| 2-Methylpentane                                      | lq             | −204.6                                                |                                                       | 290.6                                                           | 193.7                                                             |
|                                                      | g              | −174.8                                                | −5.0                                                  | 380.5                                                           | 144.2                                                             |
| 3-Methylpentane                                      | lq             | −202.4                                                |                                                       | 292.5                                                           | 190.7                                                             |
|                                                      | g              | −172.1                                                | 2.1                                                   | 379.8                                                           | 143.1                                                             |
| 2-Methyl-2,4-pentanediol                             | lq             |                                                       |                                                       |                                                                 | 236.0                                                             |
| Methyl pentanoate                                    | lq             | −514.2                                                |                                                       |                                                                 | 229.3                                                             |
| 2-Methyl-1-pentanol                                  | lq             |                                                       |                                                       |                                                                 | 248.0                                                             |
| 2-Methyl-3-pentanol                                  | lq             | −396.4                                                |                                                       |                                                                 |                                                                   |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                    | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 3-Methyl-2-pentanol          | lq             |                                            |                                            |                                                     | 275.9                                                 |
| 3-Methyl-3-pentanol          | lq             |                                            |                                            |                                                     | 293.4                                                 |
| 4-Methyl-2-pentanol          | lq             | - 394.7                                    |                                            |                                                     | 273.0                                                 |
| 2-Methyl-3-pentanone         | lq             | - 325.9                                    |                                            |                                                     |                                                       |
| 4-Methyl-2-pentanone         | lq             |                                            |                                            |                                                     | 213.3                                                 |
| 2-Methyl-1-pentene           | g              | - 59.4                                     | 77.6                                       | 382.2                                               | 135.6                                                 |
| 2-Methyl-2-pentene           | g              | - 66.9                                     | 71.2                                       | 378.4                                               | 126.6                                                 |
| 3-Methyl-1-pentene           | g              | - 49.5                                     | 86.4                                       | 376.8                                               | 142.4                                                 |
| cis-3-Methyl-2-pentene       | g              | - 62.3                                     | 73.2                                       | 378.4                                               | 126.6                                                 |
| trans-3-Methyl-2-pentene     | g              | - 63.1                                     | 71.3                                       | 381.8                                               | 126.6                                                 |
| 4-Methyl-1-pentene           | g              | - 51.3                                     | 90.0                                       | 367.7                                               | 126.5                                                 |
| cis-4-Methyl-2-pentene       | g              | - 57.5                                     | 82.1                                       | 373.3                                               | 133.6                                                 |
| trans-4-Methyl-2-pentene     | g              | - 61.5                                     | 79.6                                       | 368.3                                               | 141.4                                                 |
| Methyl 2-methylpropenoate    | lq             |                                            |                                            |                                                     | 191.2                                                 |
| 4-Methyl-3-penten-2-one      | lq             |                                            |                                            |                                                     | 212.5                                                 |
| Methyl pentyl sulfide        | g              | 122.9                                      | 35.1                                       | 450.7                                               | 163.7                                                 |
| 3-Methyl-1-phenyl-1-butanone | lq             | - 220.2                                    |                                            |                                                     |                                                       |
| Methyl phenyl sulfide        | lq             | 43.0                                       |                                            |                                                     |                                                       |
| Methyl phenyl sulfone        | c              | - 345.4                                    |                                            |                                                     |                                                       |
| Methylphosphonic acid        | c              | - 1054                                     |                                            |                                                     |                                                       |
| (±)-2-Methylpiperidine       | lq             | - 124.9                                    |                                            |                                                     |                                                       |
| 2-Methylpropanal             | lq             | - 247.4                                    |                                            |                                                     |                                                       |
|                              | g              | - 215.8                                    |                                            |                                                     |                                                       |
| N-Methylpropanamide          | lq             |                                            |                                            |                                                     | 179                                                   |
| 2-Methylpropanamine          | lq             | - 132.6                                    |                                            |                                                     | 183.2                                                 |
| 2-Methylpropane              | g              | - 134.2                                    | - 20.9                                     | 294.6                                               | 130.5 <sup>-12</sup>                                  |
| 2-Methyl-1,2-propanediamine  | lq             | - 133.9                                    |                                            |                                                     |                                                       |
| 2-Methyl-1,2-propanediol     | lq             | - 539.7                                    |                                            |                                                     |                                                       |
| 2-Methylpropanenitrile       | lq             | - 13.8                                     |                                            |                                                     |                                                       |
| 2-Methyl-1-propanethiol      | g              | - 97.3                                     | 5.6                                        | 362.9                                               | 118.3                                                 |
| 2-Methyl-2-propanethiol      | g              | - 109.6                                    | 0.7                                        | 338.0                                               | 121.0                                                 |
| 2-Methylpropanoic acid       | lq             |                                            |                                            |                                                     | 173                                                   |
| 2-Methyl-1-propanol          | lq             | - 334.7                                    |                                            | 214.7                                               | 181.2                                                 |
|                              | g              | - 283.9                                    | - 167.35                                   | 359.0                                               | 111.3                                                 |
| 2-Methyl-2-propanol          | lq             | - 359.2                                    |                                            | 193.3                                               | 219.8                                                 |
|                              | g              | - 312.5                                    | - 177.7                                    | 326.7                                               | 113.6                                                 |
| 2-Methylpropene              | g              | - 16.9                                     | 58.1                                       | 293.6                                               | 89.1                                                  |
| 2-Methylpropenoic acid       | lq             |                                            |                                            |                                                     | 161.1                                                 |
| 1-Methyl-2-propylbenzene     | lq             | - 72.5                                     |                                            |                                                     |                                                       |
| 1-Methyl-3-propylbenzene     | lq             | - 76.2                                     |                                            |                                                     |                                                       |
| 1-Methyl-4-propylbenzene     | lq             | - 75.1                                     |                                            |                                                     |                                                       |
| (2-Methylpropyl)benzene      | lq             | - 69.8                                     |                                            |                                                     | 240.6                                                 |
| Methyl propyl ether          | lq             | - 266.0                                    |                                            | 262.9                                               | 165.4                                                 |
|                              | g              | - 238.2                                    | - 109.9                                    | 349.5                                               | 112.5                                                 |
| Methyl propyl sulfide        | g              | - 82.3                                     | 18.4                                       | 371.7                                               | 117.4                                                 |
| 2-Methylpyridine             | lq             | 56.7                                       | 166.5                                      | 217.9                                               | 158.4                                                 |
|                              | g              | 99.2                                       | 177.1                                      | 325.0                                               | 100.0                                                 |
| 3-Methylpyridine             | lq             | 61.9                                       | 214.0                                      | 216.3                                               | 158.7                                                 |
|                              | g              | 106.4                                      | 184.3                                      | 325.0                                               | 99.6                                                  |
| 4-Methylpyridine             | lq             | 59.2                                       |                                            | 209.1                                               | 159.0                                                 |
| 1-Methyl-1 <i>H</i> -pyrrole | lq             | 62.4                                       |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                               | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 2-Methyl-1 <i>H</i> -pyrrole            | lq             | 23.3                                       |                                            |                                                     |                                                       |
| 3-Methyl-1 <i>H</i> -pyrrole            | lq             | 20.5                                       |                                            |                                                     |                                                       |
| <i>N</i> -Methylpyrrolidone             | lq             | -262.2                                     |                                            |                                                     | 307.8                                                 |
| 2-Methylquinoline                       | c              | 164.4                                      |                                            |                                                     |                                                       |
| Methyl salicylate                       | lq             | -531.8                                     |                                            |                                                     | 249.0                                                 |
| Methylsilane                            | g              |                                            |                                            | 256.5                                               | 65.9                                                  |
| $\alpha$ -Methylstyrene                 | g              | 113.0                                      | 208.5                                      | 383.7                                               | 145.2                                                 |
| <i>cis</i> -( $\beta$ )-Methylstyrene   | g              | 121.3                                      | 216.9                                      | 383.7                                               | 145.2                                                 |
| <i>trans</i> -( $\beta$ )-Methylstyrene | g              | 117.2                                      | 213.7                                      | 380.3                                               | 146.0                                                 |
| Methylsuccinic acid                     | c              | -958.2                                     |                                            |                                                     |                                                       |
| Methylsuccinic anhydride                | lq             | -617.6                                     |                                            |                                                     |                                                       |
| Methyl tetradecanoate                   | lq             | -743.9                                     |                                            |                                                     |                                                       |
| 2-Methylthiacyclopentane                | g              | -63.3                                      |                                            |                                                     |                                                       |
| 4-Methylthiazole                        | lq             | 68.0                                       |                                            |                                                     |                                                       |
| Methylthiirane                          | g              | 45.8                                       |                                            |                                                     |                                                       |
| 2-Methylthiophene                       | lq             | 44.6                                       |                                            |                                                     | 149.8                                                 |
|                                         | g              | 83.5                                       | 122.9                                      | 320.6                                               | 95.4                                                  |
| 3-Methylthiophene                       | lq             | 43.1                                       |                                            |                                                     |                                                       |
|                                         | g              | 82.6                                       | 121.8                                      | 321.3                                               | 94.9                                                  |
| Methyl <i>p</i> -tolyl sulfone          | c              | -372.8                                     |                                            |                                                     |                                                       |
| 5-Methyluracil                          | c              | -462.8                                     |                                            |                                                     |                                                       |
| Methylurea                              | c              | -332.8                                     |                                            |                                                     |                                                       |
| Morphine monohydrate                    | c              | -711.7                                     |                                            |                                                     |                                                       |
| Morpholine                              | lq             |                                            |                                            |                                                     | 164.8                                                 |
| Murexide                                | c              | -1212.1                                    |                                            |                                                     |                                                       |
| Naphthalene                             | c              | 77.9                                       | 201.6                                      | 167.4                                               | 165.7                                                 |
|                                         | g              | 150.6                                      | 224.1                                      | 333.1                                               | 131.9                                                 |
| 1-Naphthaleneacetic acid                | c              | -359.2                                     |                                            |                                                     |                                                       |
| 2-Naphthaleneacetic acid                | c              | -371.9                                     |                                            |                                                     |                                                       |
| 1-Naphthoic acid                        | c              | 333.5                                      |                                            |                                                     |                                                       |
| 2-Naphthoic acid                        | c              | -346.1                                     |                                            |                                                     |                                                       |
| 1-Naphthol                              | c              | -121.0                                     |                                            |                                                     | 166.9                                                 |
| 2-Naphthol                              | lq             | -124.2                                     |                                            |                                                     |                                                       |
| 1,4-Naphthoquinone                      | c              | -183.4                                     |                                            |                                                     |                                                       |
| 1-Naphthyl acetate                      | c              | -288.2                                     |                                            |                                                     |                                                       |
| 2-Naphthyl acetate                      | c              | -304.3                                     |                                            |                                                     |                                                       |
| 1-Naphthylamine                         | c              | 67.8                                       |                                            |                                                     |                                                       |
| 2-Naphthylamine                         | c              | 59.7                                       |                                            |                                                     |                                                       |
| Nicotine                                | lq             | 39.3                                       |                                            |                                                     |                                                       |
| Nitrilotriacetic acid                   | c              | -1311.9                                    | -1307.5                                    |                                                     |                                                       |
| Nitroacetone                            | lq             | -278.6                                     |                                            |                                                     |                                                       |
| 2-Nitroaniline                          | c              | -26.1                                      | 178.2                                      | 176.2                                               | 166.0                                                 |
| 3-Nitroaniline                          | c              | -38.3                                      | 174.1                                      | 176.2                                               | 158.8                                                 |
| 4-Nitroaniline                          | c              | -42.0                                      | 151.0                                      | 176.2                                               | 167.0                                                 |
| Nitrobenzene                            | lq             | 12.5                                       | 146.2                                      | 224.3                                               | 185.8                                                 |
| 2-Nitrobenzoic acid                     | c              | -378.5                                     | -196.4                                     | 208.4                                               |                                                       |
| 3-Nitrobenzoic acid                     | c              | -394.7                                     | -220.5                                     | 205.0                                               |                                                       |
| 4-Nitrobenzoic acid                     | c              | -392.2                                     | -222.0                                     | 210.0                                               | 181.2                                                 |
| 3-Nitrobiphenyl                         | c              | 65.1                                       |                                            |                                                     |                                                       |
| 4-Nitrobiphenyl                         | c              | 40.5                                       |                                            |                                                     |                                                       |
| 1-Nitrobutane                           | g              | -143.9                                     | 10.1                                       | 394.5                                               | 124.9                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                   | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 2-Nitrobutane               | g              | -163.6                                     | -6.2                                       | 383.3                                               | 123.5                                                 |
| 3-Nitro-2-butanol           | lq             | -390.0                                     |                                            |                                                     |                                                       |
| N-Nitrodiethylamine         | lq             | -106.2                                     |                                            |                                                     |                                                       |
| 2-Nitrodiphenylamine        | c              | 64.4                                       |                                            |                                                     |                                                       |
| Nitroethane                 | lq             | -143.9                                     |                                            |                                                     | 134.4                                                 |
|                             | g              | -102.3                                     | -4.9                                       | 315.4                                               | 78.2                                                  |
| 2-Nitroethanol              | lq             | -350.7                                     |                                            |                                                     |                                                       |
| 2-Nitrofurane               | c              | -104.1                                     |                                            |                                                     |                                                       |
| 5-Nitrofurancarboxylic acid | c              | -516.8                                     |                                            |                                                     |                                                       |
| 1-Nitroguanidine            | c              | -92.4                                      |                                            |                                                     |                                                       |
| Nitromethane                | lq             | -113.1                                     | -14.4                                      | 171.8                                               | 106.6                                                 |
|                             | g              | -74.3                                      | -6.8                                       | 275.0                                               | 57.3                                                  |
| (Nitromethyl)benzene        | lq             | -22.8                                      |                                            |                                                     |                                                       |
| 1-Nitronaphthalene          | c              | 42.6                                       |                                            |                                                     |                                                       |
| 1-Nitroso-2-naphthol        | c              | -50.5                                      |                                            |                                                     |                                                       |
| 2-Nitroso-1-naphthol        | c              | -61.8                                      |                                            |                                                     |                                                       |
| 4-Nitroso-1-naphthol        | c              | -107.8                                     |                                            |                                                     |                                                       |
| 1-Nitropropane              | lq             | -167.2                                     |                                            |                                                     | 175.3                                                 |
|                             | g              | -123.8                                     |                                            |                                                     |                                                       |
| 2-Nitropropane              | lq             | -180.3                                     |                                            |                                                     | 170.3                                                 |
|                             | g              | -139.0                                     |                                            |                                                     |                                                       |
| 1-Nitro-2-propanone         | c              | -294.7                                     |                                            |                                                     |                                                       |
| 4-Nitrosodiphenylamine      | c              | 213.0                                      |                                            |                                                     |                                                       |
| $\beta$ -Nitrostyrene       | c              | 30.5                                       |                                            |                                                     |                                                       |
| 4-Nitrotoluene              | c              | -48.1                                      |                                            |                                                     | 172.3                                                 |
| Nonadecane                  | g              | -435.1                                     | 108.9                                      | 895.2                                               | 440.4                                                 |
| 1-Nonadecene                | g              | -309.6                                     | 196.7                                      | 891.0                                               | 429.7                                                 |
| 1-Nonanal                   | g              | -310.3                                     | -74.9                                      | 539.6                                               | 216.8                                                 |
| Nonane                      | lq             | -274.7                                     |                                            |                                                     | 284.4                                                 |
|                             | g              | -228.2                                     | 24.8                                       | 505.7                                               | 211.7                                                 |
| 1-Nonanethiol               | g              | -190.8                                     | 53.0                                       | 571.2                                               | 232.7                                                 |
| Nonanoic acid               | lq             | -659.7                                     |                                            |                                                     | 362.4                                                 |
| 1-Nonanol                   | g              | -376.3                                     | -110.5                                     | 558.6                                               | 224.3                                                 |
| 2-Nonanone                  | lq             | -397.2                                     |                                            |                                                     |                                                       |
| 5-Nonanone                  | lq             | -398.2                                     |                                            | 401.4                                               | 303.6                                                 |
| 1-Nonene                    | g              | -103.5                                     | 112.7                                      | 501.5                                               | 201.0                                                 |
| Norleucine                  | c              | -639.1                                     |                                            |                                                     |                                                       |
| Octadecane                  | c              | -567.4                                     |                                            | 480.2                                               | 485.6                                                 |
|                             | g              | -414.6                                     | 100.5                                      | 856.2                                               | 417.6                                                 |
| Octadecanoic acid           | c              | -947.7                                     |                                            |                                                     | 501.5                                                 |
| 1,8-Octadecanoic acid       | c              | -1038.1                                    |                                            |                                                     |                                                       |
| 1-Octadecene                | g              | -289.0                                     | 188.3                                      | 852.0                                               | 406.8                                                 |
| cis-9-Octadecenoic acid     | lq             | -743.5                                     |                                            |                                                     | 577.0 <sup>50</sup>                                   |
| trans-9-Octadecenoic acid   | c              | -910.9                                     |                                            |                                                     |                                                       |
| 1,7-Octadiyne               | lq             | 334.4                                      |                                            |                                                     |                                                       |
| Octafluorocyclobutane       | lq             |                                            |                                            |                                                     | 209.8 <sup>-6</sup>                                   |
|                             | g              | -1542.6                                    | -1398.8                                    | 400.4                                               | 156.2                                                 |
| Octafluoropropane           | g              | -1783.1                                    |                                            |                                                     |                                                       |
| Octafluorotoluene           | lq             | -1311.1                                    |                                            | 355.5                                               | 262.3                                                 |
| 1-Octanal                   | g              | -289.6                                     | -83.3                                      | 500.7                                               | 194.0                                                 |
| Octanamide                  | c              | -473.2                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                                                      | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------------------------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Octane                                                                         | lq             | -250.1                                     |                                            |                                                     | 254.6                                                 |
|                                                                                | g              | -208.6                                     | 16.4                                       | 466.7                                               | 188.9                                                 |
| 1-Octanenitrile                                                                | lq             | -107.3                                     |                                            |                                                     |                                                       |
| 1-Octanethiol                                                                  | g              | -44.9                                      | 44.6                                       | 582.2                                               | 209.8                                                 |
| Octanoic acid                                                                  | lq             | -636.0                                     |                                            |                                                     | 297.9                                                 |
| 1-Octanol                                                                      | lq             | -426.5                                     | -143.1                                     | 377.4                                               | 305.1                                                 |
| 2-Octanol                                                                      | lq             |                                            |                                            |                                                     | 330.1                                                 |
| 2-Octanone                                                                     | lq             | -384.5                                     | -140.3                                     | 373.8                                               | 273.3                                                 |
| 1-Octene                                                                       | lq             | -121.8                                     |                                            |                                                     | 241.0                                                 |
|                                                                                | g              | -81.4                                      | 104.2                                      | 462.5                                               | 178.1                                                 |
| <i>cis</i> -2-Octene                                                           | lq             | -135.7                                     |                                            |                                                     | 239.0                                                 |
| <i>trans</i> -2-Octene                                                         | lq             | -135.7                                     |                                            |                                                     | 239.0                                                 |
| 1-Octyne                                                                       | g              | 82.4                                       | 235.4                                      | 496.6                                               | 174.0                                                 |
| (±)-Ornithine                                                                  | c              | -652.7                                     |                                            |                                                     |                                                       |
| Oxalic acid                                                                    | c              | -821.7                                     | -697.9                                     | 109.8                                               | 91.0                                                  |
| Oxalic acid dihydrate                                                          | c              | -1492.0                                    |                                            |                                                     |                                                       |
| Oxaloyl dichloride                                                             | lq             | -367.6                                     |                                            |                                                     |                                                       |
| Oxaloyl dihydrazide                                                            | c              | -295.2                                     |                                            |                                                     |                                                       |
| Oxamic acid                                                                    | c              | -661.2                                     |                                            |                                                     |                                                       |
| Oxamide                                                                        | c              | -504.4                                     | -342.7                                     | 118.0                                               |                                                       |
| Oxazole                                                                        | g              | -5.5                                       |                                            |                                                     |                                                       |
| 2-Oxetanone                                                                    | lq             | -329.9                                     |                                            | 175.3                                               | 122.1                                                 |
| Oxindole                                                                       | c              | -172.4                                     |                                            |                                                     |                                                       |
| 2-Oxohexamethyleneimine                                                        | c              | -329.4                                     | -95.1                                      | 168.6                                               | 156.8                                                 |
| Oxomethyl (HCO)                                                                | g              | 43.1                                       | 28.0                                       | 224.7                                               | 34.6                                                  |
| 2-Oxo-1,5-pentanedioic acid                                                    | c              | -1026.2                                    |                                            |                                                     |                                                       |
| 4-Oxopentanoic acid                                                            | c              | -697.1                                     |                                            |                                                     |                                                       |
| 2-Oxopropanoic acid                                                            | lq             | -584.5                                     | -463.4                                     | 179.5                                               |                                                       |
| 8-Oxypurine                                                                    | c              | -64.4                                      |                                            |                                                     |                                                       |
| Papaverine                                                                     | c              | -502.3                                     |                                            |                                                     |                                                       |
| Paraformaldehyde                                                               | c              | -177.6                                     |                                            |                                                     |                                                       |
| Paraldehyde                                                                    | lq             | -687.0                                     |                                            |                                                     |                                                       |
| Pentachloroethane                                                              | lq             | -187.6                                     |                                            |                                                     | 173.8                                                 |
|                                                                                | g              | -142.0                                     | -70.3                                      | 381.5                                               | 118.1                                                 |
| Pentachlorofluoroethane                                                        | g              | -317.2                                     | -234.0                                     | 391.8                                               |                                                       |
| Pentachlorophenol                                                              | c              | -292.4                                     | -144.1                                     | 251.9                                               | 202.0                                                 |
| Pentacyclo[4.2.0.0 <sup>2,5</sup> .0 <sup>3,8</sup> .0 <sup>4,7</sup> ]-octane | c              | 541.8                                      |                                            |                                                     |                                                       |
| Pentadecane                                                                    | g              | -352.8                                     | 75.2                                       | 739.4                                               | 349.0                                                 |
| Pentadecanoic acid                                                             | c              | -861.7                                     |                                            |                                                     | 443.3                                                 |
| 1-Pentadecene                                                                  | g              | -227.2                                     | 163.1                                      | 735.2                                               | 338.2                                                 |
| 1-Pentadecyne                                                                  | g              | -61.8                                      | 293.9                                      | 719.3                                               | 33.41                                                 |
| 1,2-Pentadiene                                                                 | g              | 140.7                                      | 210.4                                      | 333.5                                               | 105.4                                                 |
| <i>cis</i> -1,3-Pentadiene                                                     | g              | 81.5                                       | 145.8                                      | 324.3                                               | 94.6                                                  |
| <i>trans</i> -1,3-Pentadiene                                                   | g              | 76.5                                       | 146.73                                     | 319.7                                               | 103.3                                                 |
| 1,4-Pentadiene                                                                 | g              | 105.7                                      | 170.3                                      | 333.5                                               | 105.0                                                 |
| 2,3-Pentadiene                                                                 | g              | 133.1                                      | 205.9                                      | 324.7                                               | 101.3                                                 |
| Pentaerythritol                                                                | c              | -920.6                                     | -613.8                                     | 198.1                                               | 190.4                                                 |
| Pentaerythritol tetranitrate                                                   | c              | -538.6                                     |                                            |                                                     |                                                       |
| Pentafluorobenzoic acid                                                        | c              | -1239.6                                    |                                            |                                                     |                                                       |
| Pentafluoroethane                                                              | g              | -1104.6                                    | -1029.3                                    | 333.7                                               | 95.7                                                  |



**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                    | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Pentafluorophenol            | c              | −1024.1                                    |                                            |                                                     |                                                       |
| 2,3,4,5,6-Pentafluorotoluene | lq             | −883.8                                     |                                            | 306.4                                               | 225.8                                                 |
| Pentamethylbenzene           | c              | −133.6                                     |                                            |                                                     |                                                       |
|                              | g              | −74.5                                      | 123.3                                      | 443.9                                               | 216.5                                                 |
| Pentamethylbenzoic acid      | c              | −536.1                                     |                                            |                                                     |                                                       |
| Pentanal                     | g              | −228.5                                     | −108.3                                     | 383.0                                               | 125.4                                                 |
| Pentanamide                  | c              | −379.5                                     |                                            |                                                     |                                                       |
| 1-Pentanamine                | lq             |                                            |                                            |                                                     | 218.0                                                 |
| Pentane                      | lq             | −173.5                                     | −9.3                                       | 262.7                                               | 167.2                                                 |
|                              | g              | −146.9                                     | −8.4                                       | 349.0                                               | 120.2                                                 |
| 1,5-Pentanediol              | lq             | −531.5                                     |                                            |                                                     | 321.3                                                 |
| 2,4-Pentanedione             | lq             | −423.8                                     |                                            |                                                     | 208.2                                                 |
|                              | g              | −380.6                                     |                                            | 397.9                                               | 120.1                                                 |
| 1,5-Pentanedithiol           | g              | −71.0                                      |                                            |                                                     |                                                       |
| Pentanenitrile               | lq             | −33.1                                      |                                            |                                                     | 180                                                   |
| 1-Pentanethiol               | lq             | −151.3                                     |                                            |                                                     |                                                       |
| Pentanoic acid               | lq             | −559.4                                     |                                            | 259.8                                               | 210.3                                                 |
|                              | g              | −491.9                                     | −357.2                                     | 439.8                                               |                                                       |
| 1-Pentanol                   | lq             | −351.6                                     |                                            |                                                     | 208.1                                                 |
|                              | g              | −294.7                                     | −146.0                                     | 402.5                                               | 133.1                                                 |
| 2-Pentanol                   | lq             | −365.2                                     |                                            |                                                     |                                                       |
|                              | g              | −311.0                                     |                                            |                                                     |                                                       |
| 3-Pentanol                   | lq             | −368.9                                     |                                            |                                                     | 239.7                                                 |
|                              | g              | −311.4                                     | −158.2                                     | 382.0                                               |                                                       |
| 2-Pentanone                  | lq             | −297.3                                     |                                            |                                                     | 184.1                                                 |
|                              | g              | −259.0                                     | −137.1                                     | 376.2                                               | 121.0                                                 |
| 3-Pentanone                  | lq             | −296.5                                     |                                            | 266.0                                               | 190.9                                                 |
| 1-Pentene                    | lq             | −46.0                                      |                                            | 262.6                                               | 154.0                                                 |
|                              | g              | −21.2                                      | 79.1                                       | 345.8                                               | 109.6                                                 |
| cis-2-Pentene                | lq             | −53.7                                      |                                            | 258.6                                               | 151.7                                                 |
|                              | g              | −27.6                                      | 71.8                                       | 346.3                                               | 101.8                                                 |
| trans-2-Pentene              | lq             | −58.2                                      |                                            | 256.5                                               | 157.0                                                 |
|                              | g              | −31.9                                      | 69.9                                       | 340.4                                               | 108.5                                                 |
| cis-2-Pentenitrile           | lq             | 71.8                                       |                                            |                                                     |                                                       |
| trans-2-Pentenitrile         | lq             | 74.9                                       |                                            |                                                     |                                                       |
| trans-3-Pentenitrile         | lq             | 80.9                                       |                                            |                                                     |                                                       |
| 2-Pentenoic acid             | lq             | −446.4                                     |                                            |                                                     |                                                       |
| 3-Pentenoic acid             | lq             | −434.8                                     |                                            |                                                     |                                                       |
| 4-Pentenoic acid             | lq             | −430.6                                     |                                            |                                                     |                                                       |
| cis-3-Penten-1-yne           | lq             | 226.5                                      |                                            |                                                     |                                                       |
| trans-3-Penten-1-yne         | lq             | 228.2                                      |                                            |                                                     |                                                       |
| Pentyl acetate               | lq             |                                            |                                            |                                                     | 261.0                                                 |
| 1-Pentyne                    | g              | 144.4                                      | 210.3                                      | 329.8                                               | 106.7                                                 |
| 2-Pentyne                    | g              | 128.9                                      | 194.2                                      | 331.8                                               | 98.7                                                  |
| Perfluoropiperidine          | lq             | −2020.5                                    | −1768.5                                    | 393.4                                               | 296.8                                                 |
| Perylene                     | c              | 182.8                                      |                                            |                                                     |                                                       |
| α-Phellandrene               | lq             | 41.3                                       |                                            |                                                     |                                                       |
| Phenanthrene                 | c              | 116.2                                      | 268.3                                      | 215.1                                               | 220.6                                                 |
| 9,10-Phenanthrene-dione      | c              | −154.7                                     |                                            |                                                     |                                                       |
| Phenazine                    | c              | 237.0                                      |                                            |                                                     |                                                       |
| Phenol                       | c              | −165.1                                     | −50.4                                      | 144.0                                               | 127.4                                                 |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|--------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
|                          | lq             |                                            |                                            |                                                     | 199.8 <sup>41</sup>                                   |
|                          | g              | − 96.4                                     | − 32.9                                     | 315.6                                               | 103.6                                                 |
| Phenoxyacetic acid       | c              | − 513.8                                    |                                            |                                                     |                                                       |
| Phenyl acetate           | lq             | − 334.9                                    |                                            |                                                     |                                                       |
| Phenylacetic acid        | c              | − 398.7                                    |                                            |                                                     |                                                       |
| Phenylacetylene          | g              | 327.3                                      | 363.5                                      | 321.7                                               | 114.9                                                 |
| (±)-3-Phenyl-2-alanine   | c              | − 466.9                                    | − 211.7                                    | 213.6                                               | 203.0                                                 |
| Phenyl benzoate          | c              | − 241.0                                    |                                            |                                                     |                                                       |
| Phenylboron dichloride   | lq             | − 299.4                                    |                                            |                                                     |                                                       |
| 1-Phenylcyclohexene      | lq             | − 16.8                                     |                                            |                                                     |                                                       |
| Phenylcyclopropane       | lq             | 100.3                                      |                                            |                                                     |                                                       |
| N-Phenyldiacetamide      | c              | − 362.5                                    |                                            |                                                     |                                                       |
| 1,3-Phenylenediamine     | c              | − 7.8                                      |                                            | 154.5                                               | 159.6                                                 |
| Phenyl formate           | lq             | − 268.7                                    |                                            |                                                     |                                                       |
| N-Phenylglycine          | c              | − 402.5                                    |                                            |                                                     |                                                       |
| (±)-2-Phenylglycine      | c              | − 431.8                                    |                                            |                                                     |                                                       |
| Phenylhydrazine          | lq             | 141.0                                      |                                            |                                                     | 217.0                                                 |
| Phenyl 2-hydroxybenzoate | c              | − 436.6                                    |                                            |                                                     |                                                       |
| Phenylmethanethiol       | lq             | 43.5                                       |                                            |                                                     |                                                       |
| Phenylmethyl acetate     | lq             |                                            |                                            |                                                     | 148.5                                                 |
| N-Phenyl-2-naphthylamine | c              | 159.8                                      |                                            |                                                     |                                                       |
| 1-Phenyl-1-propanone     | lq             | − 167.2                                    |                                            |                                                     |                                                       |
| 1-Phenyl-2-propanone     | lq             | − 151.9                                    |                                            |                                                     |                                                       |
| 1-Phenylpyrrole          | c              | 154.3                                      |                                            |                                                     |                                                       |
| 2-Phenylpyrrole          | c              | 139.2                                      |                                            |                                                     |                                                       |
| Phenylsuccinic acid      | c              | − 841.0                                    |                                            |                                                     |                                                       |
| S-Phenyl thioacetate     | lq             | − 122.0                                    |                                            |                                                     |                                                       |
| Phenyl vinyl ether       | lq             | − 26.2                                     |                                            |                                                     |                                                       |
| Phosgene                 | g              | − 220.9                                    | − 206.8                                    | 283.8                                               | 57.7                                                  |
| Phthalamide              | c              | − 433.1                                    |                                            |                                                     |                                                       |
| 1,2-Phthalic acid        | c              | − 782.0                                    | − 591.6                                    | 207.9                                               | 188.3                                                 |
| 1,3-Phthalic acid        | c              | − 803.0                                    |                                            |                                                     |                                                       |
| 1,4-Phthalic acid        | c              | − 816.1                                    |                                            |                                                     |                                                       |
| Phthalic anhydride       | c              | − 460.1                                    | − 331.0                                    | 180.0                                               | 160.0                                                 |
| Phthalonitrile           | c              | 280.6                                      |                                            |                                                     |                                                       |
| Picric acid              | c              | − 214.4                                    |                                            |                                                     |                                                       |
| α-Pinene                 | lq             | − 16.4                                     |                                            |                                                     |                                                       |
| β-Pinene                 | lq             | − 7.7                                      |                                            |                                                     |                                                       |
| Piperazine               | c              | − 45.6                                     | 240.2                                      | 85.8                                                |                                                       |
| 2,5-Piperazinedione      | c              | − 446.5                                    |                                            |                                                     |                                                       |
| Piperidine               | lq             | − 86.4                                     |                                            | 210.0                                               | 179.9                                                 |
| 2-Piperidone             | c              | − 306.6                                    | − 112.1                                    | 164.9                                               | (lq 307.8)                                            |
| L-Proline                | c              | 515.2                                      |                                            |                                                     |                                                       |
| Propadiene               | g              | 190.5                                      | 202.4                                      | 243.9                                               | 59.0                                                  |
| Propanal                 | lq             | − 215.3                                    |                                            |                                                     | 137.2                                                 |
|                          | g              | − 185.6                                    | − 130.5                                    | 304.5                                               | 80.7                                                  |
| Propanamide              | c              | − 338.2                                    |                                            |                                                     |                                                       |
| Propane                  | lq             |                                            |                                            |                                                     | 98.3 <sup>−43</sup>                                   |
|                          | g              | − 103.8                                    | − 23.4                                     | 270.2                                               | 73.6                                                  |
| Propanediamide           | c              | − 546.1                                    |                                            |                                                     |                                                       |
| (±)-1,2-Propanediamine   | lq             | − 97.8                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                              | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 1,2-Propanediol                        | lq             | -485.7                                     |                                            |                                                     | 190.8                                                 |
| 1,3-Propanediol                        | lq             | -464.9                                     |                                            |                                                     |                                                       |
| 1,2-Propanedione                       | lq             | -309.1                                     |                                            |                                                     |                                                       |
| Propanedinitrile                       | lq             | 186.4                                      |                                            |                                                     |                                                       |
| 1,2-Propanedithiol                     | lq             | -79.4                                      |                                            |                                                     |                                                       |
| 1,3-Propanedithiol                     | lq             | -79.4                                      |                                            |                                                     |                                                       |
| Propanenitrile                         | lq             | 15.5                                       | 89.2                                       | 189.3                                               | 119.3                                                 |
| 1-Propanethiol                         | lq             | -99.9                                      |                                            | 242.5                                               | 144.6                                                 |
|                                        | g              | -67.9                                      | 2.2                                        | 336.4                                               | 94.8                                                  |
| 2-Propanethiol                         | lq             | -105.0                                     |                                            | 233.5                                               | 145.3                                                 |
|                                        | g              | -76.2                                      | -2.6                                       | 324.3                                               | 96.0                                                  |
| 1,2,3-Propanetriol tris(acetate)       | lq             | -1330.8                                    |                                            | 458.3                                               | 384.7                                                 |
| Propanoic acid                         | lq             | -510.7                                     | -383.5                                     | 191.0                                               | 152.8                                                 |
| Propanoic anhydride                    | lq             | -679.1                                     | -475.6                                     |                                                     | 235.0                                                 |
| 1-Propanol                             | lq             | -302.6                                     | -170.6                                     | 193.6                                               | 143.7                                                 |
|                                        | g              | -255.1                                     | -161.8                                     | 322.7                                               | 85.6                                                  |
| 2-Propanol                             | lq             | -318.1                                     | -180.3                                     | 181.1                                               | 155.0                                                 |
|                                        | g              | -272.6                                     | -173.4                                     | 309.2                                               | 89.3                                                  |
| 2-Propenal                             | g              | -85.8                                      | -64.6                                      |                                                     |                                                       |
| Propene                                | g              | 20.0                                       | 62.8                                       | 266.6                                               | 64.3                                                  |
| trans-1-Propene-1,2-dicarboxylic acid  | c              | -824.4                                     |                                            |                                                     |                                                       |
| 2-Propenenitrile                       | lq             | 147.1                                      |                                            |                                                     | 108.8                                                 |
|                                        | g              | 180.6                                      | 195.4                                      | 274.1                                               | 63.8                                                  |
| cis-1,2,3-Propenetri-carboxylic acid   | c              | -1224.7                                    |                                            |                                                     |                                                       |
| trans-1,2,3-Propenetri-carboxylic acid | c              | -1233.0                                    |                                            |                                                     |                                                       |
| 2-Propenoic acid                       | lq             | -383.8                                     |                                            |                                                     | 145.7                                                 |
|                                        | g              | -336.5                                     | -286.3                                     | 315.2                                               | 77.8                                                  |
| 2-Propen-1-ol                          | lq             | -171.8                                     |                                            |                                                     | 138.9                                                 |
|                                        | g              | -124.5                                     | -71.3                                      | 307.6                                               | 76.0                                                  |
| 2-Propenyl acetate                     | lq             | -386.2                                     |                                            |                                                     | 184.1                                                 |
| cis-1-Propenylbenzene                  | g              | 121.3                                      | 216.9                                      | 383.7                                               | 145.2                                                 |
| trans-1-Propenylbenzene                | g              | 117.2                                      | 213.7                                      | 380.3                                               | 146.0                                                 |
| 2-Propenylbenzene                      | lq             | 88.0                                       |                                            |                                                     |                                                       |
| Propyl acetate                         | lq             |                                            |                                            |                                                     | 196.2                                                 |
| Propylamine                            | lq             | -101.5                                     |                                            |                                                     | 162.5                                                 |
|                                        | g              | -70.2                                      | 39.8                                       | 325.1                                               | 91.2                                                  |
| Propylbenzene                          | lq             | -38.3                                      |                                            | 287.8                                               | 214.7                                                 |
|                                        | g              | 7.9                                        | 137.2                                      | 400.7                                               | 152.3                                                 |
| Propylcarbamate                        | c              | -552.6                                     |                                            |                                                     |                                                       |
| Propylchloroacetate                    | lq             | -515.6                                     |                                            |                                                     |                                                       |
| Propylchlorocarbonate                  | g              | -492.7                                     |                                            |                                                     |                                                       |
| Propylcyclohexane                      | lq             | -237.4                                     |                                            | 311.9                                               | 242.0                                                 |
|                                        | g              | -192.5                                     | 47.3                                       | 419.5                                               | 184.2                                                 |
| Propylcyclopentane                     | lq             | -188.8                                     |                                            | 310.8                                               | 216.8                                                 |
|                                        | g              | -147.1                                     | 52.6                                       | 417.3                                               | 154.6                                                 |
| Propylene carbonate                    | lq             | -613.2                                     |                                            |                                                     | 218.6                                                 |
| Propylene oxide                        | lq             | -123.0                                     |                                            | 196.5                                               | 120.4                                                 |
|                                        | g              | -94.7                                      | -25.8                                      | 286.9                                               | 72.6                                                  |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                        | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Propyl formate                   | lq             | -500.3                                     |                                            |                                                     | 171.4                                                 |
| Propyl nitrate                   | g              | -173.9                                     | -27.3                                      | 385.4                                               | 121.3                                                 |
| S-Propyl thioacetate             | lq             | -294.1                                     |                                            |                                                     |                                                       |
| Propyl trichloroacetate          | lq             | -513.0                                     |                                            |                                                     |                                                       |
| Propyl vinyl ether               | lq             | -190.9                                     |                                            |                                                     |                                                       |
| 2-Propynyl-1-amine               | lq             | 205.7                                      |                                            |                                                     |                                                       |
| Propyne                          | g              | 184.9                                      | 194.4                                      | 248.1                                               | 60.7                                                  |
| 2-Propynoic acid                 | lq             | -193.2                                     |                                            |                                                     |                                                       |
| 1 <i>H</i> -Purine               | c              | 169.4                                      |                                            |                                                     |                                                       |
| Pyrazine                         | c              | 139.8                                      |                                            |                                                     |                                                       |
| 1 <i>H</i> -Pyrazole             | c              | 116.0                                      |                                            |                                                     |                                                       |
|                                  | lq             | 105.4                                      |                                            |                                                     |                                                       |
| Pyrene                           | c              | 125.5                                      |                                            | 224.9                                               | 229.7                                                 |
| Pyridazine                       | lq             | 224.8                                      |                                            |                                                     |                                                       |
| Pyridine                         | lq             | 100.2                                      | 181.3                                      | 177.9                                               | 132.7                                                 |
|                                  | g              | 140.4                                      | 190.2                                      | 282.8                                               | 78.1                                                  |
| 3-Pyridinecarbonitrile           | c              | 193.4                                      |                                            |                                                     |                                                       |
| 3-Pyridinecarboxylic acid        | c              | -344.9                                     |                                            |                                                     |                                                       |
| Pyrimidine                       | lq             | 145.9                                      |                                            |                                                     |                                                       |
| 1 <i>H</i> -Pyrrole              | lq             | 63.1                                       |                                            | 156.4                                               | 127.7                                                 |
| Pyrrole-2-carboxaldehyde         | c              | -106.4                                     |                                            |                                                     |                                                       |
| Pyrrole-2-carboldoxime           | c              | 12.1                                       |                                            |                                                     |                                                       |
| Pyrrolidine                      | lq             | -41.0                                      |                                            | 204.1                                               | 156.6                                                 |
|                                  | g              | -3.6                                       | 114.7                                      | 309.5                                               | 81.1                                                  |
| (±)-2-Pyrrolidinecarboxylic acid | c              | -524.2                                     |                                            |                                                     |                                                       |
| 2-Pyrrolidone                    | c              | -286.2                                     |                                            |                                                     | 164.4                                                 |
| Quinhydrone                      | c              | -82.8                                      | -323.0                                     | 325.9                                               | 277.0                                                 |
| Quinidine                        | c              | -160.3                                     |                                            |                                                     |                                                       |
| Quinine                          | c              | -155.2                                     |                                            |                                                     |                                                       |
| Quinoline                        | lq             | 141.2                                      | 275.7                                      | 217.2                                               | 194.9                                                 |
| Raffinose                        | c              | -3184                                      |                                            |                                                     |                                                       |
| L-(+)-Rhamnose                   | c              | -1073.2                                    |                                            |                                                     |                                                       |
| D-(-)-Ribose                     | c              | -1047.2                                    |                                            |                                                     |                                                       |
| Salicylaldehyde                  | lq             | -279.9                                     |                                            |                                                     | 222 <sup>18</sup>                                     |
| Salicylaldoxime                  | c              | -183.7                                     |                                            |                                                     |                                                       |
| Salicylic acid                   | c              | -589.5                                     | -418.1                                     | 178.2                                               |                                                       |
| Semicarbazide std. state         | aq             | -166.9                                     | -40.6                                      | 297.9                                               |                                                       |
| (-)-Serine                       | c              | -732.7                                     |                                            |                                                     |                                                       |
| (±)-Serine                       | c              | -739.0                                     |                                            |                                                     |                                                       |
| L-(-)-Sorbitose                  | c              | -1271.5                                    | -908.4                                     | 220.9                                               |                                                       |
| 5,5'-Spirobis(1,3-dioxane)       | c              | -702.1                                     |                                            |                                                     |                                                       |
| Spiro[2.2]pentane                | lq             | 157.5                                      |                                            | 193.7                                               | 134.5                                                 |
|                                  | g              | 185.2                                      | 265.3                                      | 282.2                                               | 88.1                                                  |
| cis-Stilbene                     | lq             | 183.3                                      |                                            |                                                     |                                                       |
| trans-Stilbene                   | c              | 136.9                                      | 317.6                                      | 251.0                                               |                                                       |
| (-)-Strychnine                   | c              | -171.5                                     |                                            |                                                     |                                                       |
| Styrene                          | lq             | 103.8                                      | 202.4                                      | 237.6                                               | 182.0                                                 |
|                                  | g              | 147.9                                      | 213.8                                      | 345.1                                               | 122.1                                                 |
| Succinic acid                    | c              | -940.5                                     | -747.4                                     | 167.3                                               | 153.1                                                 |
| Succinic acid monoamide          | c              | -581.2                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                               | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Succinic anhydride                      | c              | − 608.6                                    |                                            |                                                     |                                                       |
| Succinimide                             | c              | − 459.0                                    |                                            |                                                     |                                                       |
| Succinonitrile                          | lq             | 139.7                                      |                                            | 191.6                                               | 145.6                                                 |
| (+)-Sucrose                             | c              | − 2226.1                                   | − 1544.7                                   | 360.2                                               |                                                       |
| (±)-Tartaric acid                       | c              | − 1290.8                                   |                                            |                                                     |                                                       |
| (−)-Tartaric acid                       | c              | − 1282.4                                   |                                            |                                                     |                                                       |
| meso-Tartaric acid                      | c              | − 1279.9                                   |                                            |                                                     |                                                       |
| α-Terpinene                             | g              | − 20.5                                     |                                            |                                                     |                                                       |
| 1,1,2,2,-Tetrabromoethane               | lq             |                                            |                                            |                                                     | 165.7                                                 |
| Tetrabromoethylene                      | g              |                                            |                                            | 387.1                                               | 102.7                                                 |
| Tetrabromomethane                       | c              | 29.4                                       | 47.7                                       | 212.5                                               | 144.3                                                 |
|                                         | g              | 83.9                                       | 67.0                                       | 358.1                                               | 91.2                                                  |
| Tetrabutyltin                           | lq             | − 304.6                                    |                                            |                                                     |                                                       |
| Tetracene                               | c              | 158.8                                      |                                            |                                                     |                                                       |
| Tetrachloro-1,4-benzo-quinone           | c              | − 288.7                                    |                                            |                                                     |                                                       |
| 1,1,2,2,-Tetrachloro-1,2-difluoroethane | lq             |                                            |                                            |                                                     | 178.6                                                 |
|                                         | g              | − 489.9                                    | − 407.1                                    | 382.8                                               | 123.4                                                 |
| 1,1,1,2-Tetrachloroethane               | lq             |                                            |                                            |                                                     | 153.8                                                 |
|                                         | g              | − 149.4                                    | − 80.3                                     | 355.9                                               | 102.7                                                 |
| 1,1,2,2,-Tetrachloroethane              | lq             | − 195.0                                    | − 95.0                                     | 246.9                                               | 162.3                                                 |
|                                         | g              | − 149.2                                    | − 85.6                                     | 362.7                                               | 100.8                                                 |
| Tetrachloroethylene                     | lq             | − 50.6                                     |                                            |                                                     | 143.4                                                 |
|                                         | g              | − 10.9                                     | 3.0                                        | 266.9                                               |                                                       |
| Tetrachloromethane                      | lq             | − 128.2                                    | − 62.6                                     | 216.2                                               | 130.7                                                 |
|                                         | g              | − 95.7                                     | − 53.6                                     | 309.9                                               | 83.4                                                  |
| 1,1,1,3-Tetrachloropropane              | lq             | − 207.8                                    |                                            |                                                     |                                                       |
| 1,2,2,3-Tetrachloropropane              | lq             | − 251.8                                    |                                            |                                                     |                                                       |
| 1,1,2,2-Tetracyanocyclopropane          | c              | 590                                        |                                            |                                                     |                                                       |
| Tetracyanoethylene                      | c              | 623.8                                      |                                            |                                                     |                                                       |
| Tetracyanomethane                       | c              | 611.6                                      |                                            |                                                     |                                                       |
| Tetradecane                             | g              | − 332.1                                    | 66.9                                       | 700.4                                               | 326.1                                                 |
| Tetradecanoic acid                      | c              | − 833.5                                    |                                            |                                                     | 432.0                                                 |
| 1-Tetradecanol                          | c              | − 629.6                                    |                                            |                                                     | 388.0                                                 |
| 1-Tetradecene                           | g              | − 206.5                                    | 154.8                                      | 696.2                                               | 315.3                                                 |
| Tetraethylene glycol                    | lq             | − 981.6                                    |                                            |                                                     | 428.8                                                 |
| Tetraethylgermanium                     | lq             | − 210.5                                    |                                            |                                                     |                                                       |
| Tetraethyllead                          | lq             | 52.7                                       | 336.4                                      | 464.6                                               | 307.4                                                 |
| Tetraethylsilane                        | lq             |                                            |                                            |                                                     | 298.1                                                 |
| Tetraethyltin                           | lq             | − 95.8                                     |                                            |                                                     |                                                       |
| 1,1,1,2-Tetrafluoroethane               | g              | − 895.8                                    | − 826.2                                    | 316.2                                               | 86.3                                                  |
| Tetrafluoroethylene                     | g              | − 658.9                                    | − 623.7                                    | 300.0                                               | 80.5                                                  |
| Tetrafluoromethane                      | g              | − 933.6                                    | − 888.3                                    | 261.6                                               | 61.0                                                  |
| 2,2,3,3-Tetrafluoro-1-propanol          | g              | − 1061.3                                   |                                            |                                                     |                                                       |
| Tetrahydrofuran                         | lq             | − 216.2                                    |                                            | 204.3                                               | 124.0                                                 |
|                                         | g              | − 184.2                                    |                                            | 302.4                                               | 76.3                                                  |
| Tetrahydro-2-furanmethanol              | lq             | − 435.6                                    |                                            |                                                     | 181.2                                                 |
| 1,2,3,4-Tetrahydronaphthalene           | lq             | − 29.2                                     |                                            |                                                     | 217                                                   |
| 5,6,7,8-Tetrahydro-1-naphthol           | c              | − 285.3                                    |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                          | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Tetrahydro-2 <i>H</i> -pyran       | lq             | −258.3                                     |                                            |                                                     | 156.5                                                 |
| Tetrahydro-2 <i>H</i> -pyran-2-one | lq             | −436.7                                     |                                            |                                                     |                                                       |
| 1,2,3,6-Tetrahydropyridine         | lq             | 33.5                                       |                                            |                                                     |                                                       |
| Tetrahydrothiophene                | lq             | −72.9                                      |                                            |                                                     |                                                       |
|                                    | g              | −34.1                                      | −45.8                                      | 309.6                                               | 92.5                                                  |
| Tetrahydrothiophene-1,1-dioxide    | lq             |                                            |                                            |                                                     | 180 <sup>20</sup>                                     |
| Tetraiodoethylene                  | c              | 305.0                                      |                                            |                                                     |                                                       |
| Tetraiodomethane                   | g              | 474.0                                      | 217.1                                      | 391.9                                               | 95.9                                                  |
| Tetramethylammonium bromide        | c              | −251.0                                     |                                            |                                                     |                                                       |
| Tetramethylammonium chloride       | c              | −276.4                                     |                                            |                                                     |                                                       |
| Tetramethylammonium iodide         | c              | −203.4                                     |                                            |                                                     |                                                       |
| 1,2,3,4-Tetramethylbenzene         | lq             | −90.2                                      | 106.7                                      | 290.6                                               |                                                       |
| 1,2,3,5-Tetramethylbenzene         | lq             | −96.4                                      | 98.7                                       | 416.5                                               | 240.7                                                 |
| 1,2,4,5-Tetramethylbenzene         | c              | −119.9                                     | 101.3                                      | 245.6                                               | 215.1                                                 |
| 2,3,5,6-Tetramethylbenzoic acid    | c              | −506.1                                     |                                            |                                                     |                                                       |
| 2,2,3,3-Tetramethylbutane          | c              | −269.0                                     |                                            | 273.7                                               | 239.2                                                 |
|                                    | g              | −225.6                                     | 22.0                                       | 389.4                                               | 192.5                                                 |
| 1,1,2,2-Tetramethylcyclopropane    | lq             | −119.7                                     |                                            |                                                     |                                                       |
| Tetramethyllead                    | lq             | 97.9                                       | 262.8                                      | 320.1                                               |                                                       |
|                                    | g              | 135.9                                      | 270.7                                      | 420.5                                               | 144.0                                                 |
| 2,2,3,3-Tetramethylpentane         | lq             | −278.3                                     |                                            |                                                     | 271.5                                                 |
| 2,2,3,4-Tetramethylpentane         | lq             | −277.7                                     |                                            |                                                     |                                                       |
| 2,2,4,4-Tetramethylpentane         | lq             | −280.0                                     |                                            |                                                     | 266.3                                                 |
| 2,3,3,4-Tetramethylpentane         | lq             | −277.9                                     |                                            |                                                     |                                                       |
| Tetramethylsilane                  | lq             | −264.0                                     |                                            |                                                     | 204.1                                                 |
|                                    | g              | −239.1                                     | −100.0                                     | 359.1                                               | 143.9                                                 |
| Tetramethylsuccinic acid           | c              | −1012.5                                    |                                            |                                                     |                                                       |
| Tetramethylthiacyclopropane        | c              | −83.0                                      |                                            |                                                     |                                                       |
| Tetramethyltin                     | g              | −18.8                                      |                                            |                                                     |                                                       |
| Tetranitromethane                  | lq             | 38.4                                       |                                            |                                                     |                                                       |
| 1,1,1,2-Tetraphenylethane          | c              | 223.0                                      |                                            |                                                     |                                                       |
| 1,1,2,2-Tetraphenylethane          | c              | 216.0                                      |                                            |                                                     |                                                       |
| Tetraphenylethylene                | c              | 311.5                                      |                                            |                                                     |                                                       |
| Tetraphenylhydrazine               | c              | 457.9                                      |                                            |                                                     |                                                       |
| Tetraphenylmethane                 | c              | 247.1                                      | 574.0                                      |                                                     |                                                       |
| Tetraphenyltin                     | c              | 412.1                                      |                                            |                                                     |                                                       |
| Tetrapropylgermanium               | g              | −229.7                                     |                                            |                                                     |                                                       |
| Tetrapropyltin                     | lq             | −211.3                                     |                                            |                                                     |                                                       |
| 1,2,3,4-(1 <i>H</i> )-Tetrazole    | c              | 237.0                                      |                                            |                                                     |                                                       |
| Theobromine                        | c              | −361.5                                     |                                            |                                                     |                                                       |
| 2-Thiaadamantane                   | c              | −143.5                                     |                                            |                                                     |                                                       |
| Thiacyclobutane                    | g              | 60.6                                       | 107.1                                      | 285.0                                               | 68.3                                                  |
| Thiacycloheptane                   | g              | −61.3                                      | 84.1                                       | 361.9                                               | 124.6                                                 |
| Thiacyclohexane                    | lq             | −106.3                                     |                                            | 218.2                                               | 163.3                                                 |
|                                    | g              | −63.5                                      | 53.1                                       | 323.0                                               | 109.7                                                 |
| Thiacyclopentane                   | g              | −33.8                                      | 46.0                                       | 309.4                                               | 90.9                                                  |
| Thiacyclopropane                   | g              | 82.2                                       | 96.9                                       | 255.3                                               | 53.7                                                  |
| Thianthrene                        | c              | −182.5                                     |                                            |                                                     |                                                       |
| Thiirane                           | g              | 82.0                                       | 96.8                                       | 255.2                                               | 53.3                                                  |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                         | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Thiirene                          | g              | 300.0                                      | 275.8                                      | 255.3                                               | 54.7                                                  |
| Thioacetamide                     | c              | -71.7                                      |                                            |                                                     |                                                       |
| Thioacetic acid                   | lq             | -216.9                                     |                                            |                                                     |                                                       |
|                                   | g              | -175.1                                     | -154.0                                     | 313.2                                               | 80.9                                                  |
| 1,2-Thiocresol                    | lq             | 44.2                                       |                                            |                                                     |                                                       |
| Thiohydantoic acid                | c              | -554.8                                     |                                            |                                                     |                                                       |
| Thiohydantoin                     | c              | -249.0                                     |                                            |                                                     |                                                       |
| 2-Thiolactic acid                 | lq             | -468.4                                     |                                            |                                                     |                                                       |
| Thiophene                         | lq             | 80.2                                       | 121.2                                      | 181.2                                               | 123.8                                                 |
|                                   | g              | 115.0                                      | 126.8                                      | 278.9                                               | 72.9                                                  |
| Thiophenol                        | lq             | 64.1                                       | 134.0                                      | 222.8                                               | 173.2                                                 |
|                                   | g              | 111.6                                      | 147.6                                      | 336.9                                               | 104.9                                                 |
| Thiosemicarbazide                 | c              | 25.1                                       |                                            |                                                     |                                                       |
| Thiourea                          | c              | -89.1                                      | 21.8                                       | 115.9                                               |                                                       |
|                                   | g              | 22.9                                       |                                            |                                                     |                                                       |
| (-)-Threonine                     | c              | -807.2                                     |                                            |                                                     |                                                       |
| (±)-Threonine                     | c              | -758.8                                     |                                            |                                                     |                                                       |
| Thymine                           | c              | -462.8                                     |                                            |                                                     | 150.8                                                 |
| Thymol                            | c              | -309.7                                     |                                            |                                                     |                                                       |
| Toluene                           | lq             | 12.4                                       | 113.8                                      | 221.0                                               | 157.0                                                 |
|                                   | g              | 50.4                                       | 122.0                                      | 320.7                                               | 103.6                                                 |
| 1 <i>H</i> -1,2,4-Triazol-3-amine | c              | 76.8                                       |                                            |                                                     |                                                       |
| 2,4,6-Triamino-1,3,5-triazine     | c              | -72.4                                      | 184.5                                      | 149.1                                               |                                                       |
| 2-Triazoethanol                   | lq             | 94.6                                       |                                            |                                                     |                                                       |
| Tribenzylamine                    | c              | 140.6                                      |                                            |                                                     |                                                       |
| Tribromoacetaldehyde              | lq             | -130.3                                     |                                            |                                                     |                                                       |
| Tribromochloromethane             | g              | 12.6                                       | 9.1                                        | 357.8                                               | 89.4                                                  |
| Tribromofluoromethane             | g              | -190.0                                     | -193.1                                     | 345.9                                               | 84.4                                                  |
| Tribromomethane                   | lq             | -28.5                                      | 8.0                                        | 220.9                                               | 130.7                                                 |
|                                   | g              | 23.8                                       | -5.0                                       | 330.9                                               | 71.2                                                  |
| Tributoxyborane                   | lq             | -1199.6                                    |                                            |                                                     |                                                       |
| Tributylamine                     | lq             | -281.6                                     |                                            |                                                     |                                                       |
| Tributyl phosphate                | lq             | -1456                                      |                                            |                                                     |                                                       |
| Tributylphosphine oxide           | c              | -460                                       |                                            |                                                     |                                                       |
| Trichloroacetaldehyde             | lq             | -234.5                                     |                                            |                                                     | 151.0                                                 |
| 2,2,2-Trichloroacetamide          | c              | -358.2                                     |                                            |                                                     |                                                       |
| Trichloroacetic acid              | c              | -503.3                                     |                                            |                                                     |                                                       |
| ionized                           | aq             | -517.6                                     |                                            |                                                     |                                                       |
| Trichloroacetonitrile             | g              |                                            |                                            | 336.6                                               | 96.1                                                  |
| Trichloroacetyl chloride          | lq             | -280.8                                     |                                            |                                                     |                                                       |
| Trichlorobenzoquinone             | c              | -269.9                                     |                                            |                                                     |                                                       |
| 1,1,1-Trichloroethane             | lq             | -177.4                                     |                                            | 227.4                                               | 144.3                                                 |
|                                   | g              | -144.6                                     | -76.2                                      | 323.1                                               | 93.3                                                  |
| 1,1,2-Trichloroethane             | lq             | -191.5                                     |                                            | 232.6                                               | 150.9                                                 |
|                                   | g              | -151.2                                     | -77.5                                      | 337.1                                               | 89.0                                                  |
| Trichloroethylene                 | lq             | -43.6                                      |                                            |                                                     | 124.4                                                 |
|                                   | g              | -9.0                                       | 19.9                                       | 324.8                                               | 80.3                                                  |
| Trichlorofluoromethane            | lq             | -301.3                                     | -236.8                                     | 255.4                                               | 121.6                                                 |
|                                   | g              | -268.3                                     | -249.3                                     | 309.7                                               | 78.0                                                  |
| Trichloromethane                  | lq             | -134.5                                     | 73.7                                       | 201.7                                               | 114.2                                                 |
|                                   | g              | -102.7                                     | -76.0                                      | 295.7                                               | 65.7                                                  |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                         | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|-----------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 1,2,2-Trichloropropane            | g              | -185.8                                     | -97.8                                      | 382.9                                               | 112.2                                                 |
| 1,2,3-Trichloropropane            | lq             | -230.6                                     |                                            |                                                     | 183.6                                                 |
|                                   | g              | -182.9                                     |                                            |                                                     |                                                       |
| 1,2,3-Trichloropropene            | lq             | -101.8                                     |                                            |                                                     |                                                       |
| 1,1,2-Trichlorotrifluoroethane    | lq             | -805.8                                     |                                            |                                                     | 170.1                                                 |
| 1,1,1-Tricyanoethane              | c              | 351.0                                      |                                            |                                                     |                                                       |
| Tricyanoethylene                  | c              | 439.3                                      |                                            |                                                     |                                                       |
| Tridecane                         | g              | -311.5                                     | 58.5                                       | 661.5                                               | 303.2                                                 |
| Tridecanoic acid                  | c              | -806.6                                     |                                            |                                                     |                                                       |
| 1-Tridecene                       | g              | -186.0                                     | 146.3                                      | 657.3                                               | 292.4                                                 |
| Triethanolamine                   | c              | -664.2                                     |                                            |                                                     | 389.0                                                 |
| Triethoxyborane                   | lq             | -1047.4                                    |                                            |                                                     |                                                       |
| Triethoxymethane                  | lq             | -687.3                                     |                                            |                                                     |                                                       |
| Triethylaluminum                  | lq             | -236.8                                     |                                            |                                                     |                                                       |
| Triethylamine                     | lq             | -127.7                                     |                                            |                                                     | 219.9                                                 |
|                                   | g              | -92.8                                      | 110.3                                      | 405.4                                               | 160.9                                                 |
| Triethylaminoborane               | lq             | -198.6                                     |                                            |                                                     |                                                       |
| Triethyl arsenite                 | lq             | -706.7                                     |                                            |                                                     |                                                       |
| Triethylarsine                    | lq             | 13.0                                       |                                            |                                                     |                                                       |
| Triethylbismuthine                | lq             | 169.9                                      |                                            |                                                     |                                                       |
| Triethylborane                    | lq             | -194.6                                     | 9.4                                        | 336.7                                               | 241.2                                                 |
|                                   | g              | -157.7                                     | 16.1                                       | 437.8                                               |                                                       |
| Triethylenediamine                | c              | -14.2                                      | 239.7                                      | 157.6                                               |                                                       |
| Triethylene glycol                | lq             | -804.2                                     |                                            |                                                     |                                                       |
| Triethyl phosphate                | lq             | -1243                                      |                                            |                                                     |                                                       |
| Triethylphosphine                 | lq             | -89.1                                      |                                            |                                                     |                                                       |
| Triethyl phosphite                | lq             | -861.5                                     |                                            |                                                     |                                                       |
| Triethylstibine                   | lq             | 5.0                                        |                                            |                                                     |                                                       |
| Triethylsuccinic acid             | c              | -1066.5                                    |                                            |                                                     |                                                       |
| Triethyl thiophosphate            | lq             | -972.8                                     |                                            |                                                     |                                                       |
| Trifluoroacetic acid              | lq             | -1069.9                                    |                                            |                                                     |                                                       |
| Trifluoroacetonitrile             | g              | -497.9                                     | -461.9                                     | 298.1                                               | 77.9                                                  |
| 1,1,1-Trifluoroethane             | g              | -744.6                                     | -678.3                                     | 279.9                                               | 78.2                                                  |
| 1,1,2-Trifluoroethane             | g              | -730.7                                     |                                            |                                                     |                                                       |
| 2,2,2-Trifluoroethanol            | lq             | -932.4                                     |                                            |                                                     |                                                       |
| Trifluoroethylene                 | g              | -490.4                                     | -469.5                                     | 292.6                                               | 69.2                                                  |
| Trifluoroiodoethane               | g              | -644.5                                     |                                            |                                                     |                                                       |
| Trifluoroiodomethane              | g              | -587.8                                     | -572.0                                     | 307.5                                               | 70.9                                                  |
| Trifluoromethane                  | g              | -695.4                                     | -658.9                                     | 259.6                                               | 51.1                                                  |
| (Trifluoromethyl)benzene          | g              | -599.1                                     | -511.3                                     | 372.6                                               | 130.4                                                 |
| 1,1,1-Trifluoro-2,4-pentane-dione | lq             | -1040.2                                    |                                            |                                                     |                                                       |
| 3,3,3-Trifluoropropene            | g              | -614.2                                     |                                            |                                                     |                                                       |
| Trihexylamine                     | lq             | -433.0                                     |                                            |                                                     |                                                       |
| (±)-Trihydroxyglutaric acid       | c              | -1490                                      |                                            |                                                     |                                                       |
| 2,4,6-Trihydroxypyrimidine        | c              | -634.7                                     |                                            |                                                     |                                                       |
| Triiodomethane                    | g              | 251.0                                      | 178.0                                      | 356.2                                               | 75.1                                                  |
| Triisopropyl phosphite            | lq             | -980.3                                     |                                            |                                                     |                                                       |
| Trimethoxyborane                  | g              | -899.1                                     |                                            |                                                     |                                                       |
| Trimethoxyethane                  | lq             | -612.0                                     |                                            |                                                     |                                                       |
| Trimethoxymethane                 | lq             | -570.0                                     |                                            |                                                     |                                                       |



**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                                    | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Trimethylacetic acid                         | lq             | − 564.4                                    |                                            |                                                     |                                                       |
| Trimethylacetic anhydride                    | lq             | − 779.9                                    |                                            |                                                     |                                                       |
| 2',4',5'-Trimethylacetophenone               | lq             | − 252.3                                    |                                            |                                                     |                                                       |
| 2',4',6'-Trimethylaceto-<br>phenone          | lq             | − 267.4                                    |                                            |                                                     |                                                       |
| Trimethylaluminum                            | lq             | − 136.4                                    | − 9.9                                      | 209.4                                               | 155.6                                                 |
| Trimethylamine                               | lq             | − 45.7                                     |                                            | 208.5                                               | 137.9                                                 |
|                                              | g              | − 23.7                                     | 98.9                                       | 287.1                                               | 91.8                                                  |
| std. state                                   | aq             | − 76.0                                     | 93.0                                       | 133.5                                               |                                                       |
| Trimethylamine-aluminum<br>chloride adduct   | c              | − 879.1                                    |                                            |                                                     |                                                       |
| Trimethylamine-borane                        | c              | − 142.5                                    | 70.7                                       | 187.0                                               |                                                       |
| Trimethylammonium ion,<br>std. state         | aq             | − 112.9                                    | 37.2                                       | 196.7                                               |                                                       |
| Trimethyl arsenite                           | lq             | − 590.8                                    |                                            |                                                     |                                                       |
| Trimethylarsine                              | g              | 11.7                                       |                                            |                                                     |                                                       |
| 1,2,3-Trimethylbenzene                       | lq             | − 58.5                                     | 107.5                                      | 267.8                                               | 216.4                                                 |
| 1,2,4-Trimethylbenzene                       | lq             | − 61.8                                     | 102.3                                      | 284.2                                               | 215.0                                                 |
| 1,3,5-Trimethylbenzene                       | lq             | − 63.4                                     | 103.9                                      | 273.6                                               | 209.3                                                 |
| 2,3,4-Trimethylbenzoic acid                  | c              | − 486.6                                    |                                            |                                                     |                                                       |
| 2,3,5-Trimethylbenzoic acid                  | c              | − 488.7                                    |                                            |                                                     |                                                       |
| 2,3,6-Trimethylbenzoic acid                  | c              | − 475.7                                    |                                            |                                                     |                                                       |
| 2,4,5-Trimethylbenzoic acid                  | c              | − 495.7                                    |                                            |                                                     |                                                       |
| 2,4,6-Trimethylbenzoic acid                  | c              | − 477.9                                    |                                            |                                                     |                                                       |
| 3,4,5-Trimethylbenzoic acid                  | c              | − 500.9                                    |                                            |                                                     |                                                       |
| 2,6,6-Trimethylbicyclo-[3.1.1]-<br>2-heptene | lq             | 16.4                                       |                                            |                                                     |                                                       |
| Trimethylbismuthine                          | g              | 192.9                                      |                                            |                                                     |                                                       |
| Trimethylborane                              | g              | − 124.3                                    | − 35.9                                     | 314.7                                               | 88.5                                                  |
| 2,2,3-Trimethylbutane                        | g              | − 204.5                                    | 4.3                                        | 383.3                                               | 164.6                                                 |
| 2,2,3-Trimethylbutane                        | lq             | − 236.5                                    |                                            | 292.2                                               | 213.5                                                 |
| 2,3,3-Trimethyl-1-butene                     | lq             | − 117.7                                    |                                            |                                                     |                                                       |
| Trimethylchlorosilane                        | lq             | − 382.8                                    | − 246.4                                    | 278.2                                               |                                                       |
|                                              | g              | − 352.8                                    | − 243.5                                    | 369.1                                               |                                                       |
| cis,cis-1,3,5-Trimethyl-<br>cyclohexane      | g              | − 215.4                                    | 33.9                                       | 390.4                                               | 179.6                                                 |
| 1,1,2-Trimethylcyclopropane                  | lq             | − 96.2                                     |                                            |                                                     |                                                       |
| Trimethylene oxide (Oxetane)                 | lq             | − 110.8                                    |                                            |                                                     |                                                       |
|                                              | g              | − 80.5                                     | − 9.8                                      | 273.9                                               |                                                       |
| Trimethylgallium                             | g              | − 46.9                                     |                                            |                                                     |                                                       |
| 2,3,5-Trimethylhexane                        | lq             | − 284.0                                    |                                            |                                                     |                                                       |
| Trimethylindium                              | g              | 170.7                                      |                                            |                                                     |                                                       |
| 2,2,3-Trimethylpentane                       | lq             | − 256.9                                    | 9.3                                        | 327.6                                               | 188.9                                                 |
|                                              | g              | − 220.0                                    | 17.1                                       | 425.2                                               |                                                       |
| 2,2,4-Trimethylpentane                       | lq             | − 259.2                                    | 6.9                                        | 328.0                                               | 239.1                                                 |
|                                              | g              | − 224.0                                    | 13.7                                       | 423.2                                               |                                                       |
| 2,3,3-Trimethylpentane                       | lq             | − 253.5                                    | 10.6                                       | 334.4                                               | 245.6                                                 |
|                                              | g              | − 216.3                                    | 18.9                                       | 431.5                                               |                                                       |
| 2,3,4-Trimethylpentane                       | lq             | − 255.0                                    | 10.7                                       | 329.3                                               | 247.3                                                 |
| 2,2,4-Trimethyl-3-pentanone                  | lq             | − 381.6                                    |                                            |                                                     |                                                       |
| 2,4,4-Trimethyl-1-pentene                    | lq             | − 145.9                                    | 86.4                                       | 306.3                                               |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                        | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| 2,4,4-Trimethyl-2-pentene        | lq             | -142.4                                     | 88.0                                       | 311.7                                               |                                                       |
| Trimethylphosphine               | lq             | -122.2                                     |                                            |                                                     |                                                       |
| Trimethylphosphine oxide         | c              | -477.8                                     |                                            |                                                     |                                                       |
| Trimethyl phosphite              | lq             | -741.0                                     |                                            |                                                     |                                                       |
| Trimethylsilane                  | g              |                                            |                                            | 331.0                                               | 117.9                                                 |
| Trimethylsilanol                 | lq             | -545.0                                     |                                            |                                                     |                                                       |
| Trimethylstibine                 | g              | 32.2                                       |                                            |                                                     |                                                       |
| Trimethylsuccinic acid           | c              | -1000.8                                    |                                            |                                                     |                                                       |
| Trimethylsuccinic anhydride      | c              | -688.3                                     |                                            |                                                     |                                                       |
| Trimethylthiacyclopropane        | lq             | -60.5                                      |                                            |                                                     |                                                       |
| Trimethyltin bromide             | lq             | -185.4                                     |                                            |                                                     |                                                       |
| Trimethyltin chloride            | lq             | -213.0                                     |                                            |                                                     |                                                       |
| Trimethylurea                    | c              | -330.5                                     |                                            |                                                     |                                                       |
| Trinitroacetonitrile             | lq             | 183.7                                      |                                            |                                                     |                                                       |
| 2,4,6-Trinitroanisole            | c              | -157.3                                     |                                            |                                                     |                                                       |
| 1,3,5-Trinitrobenzene            | c              | -37.2                                      |                                            |                                                     |                                                       |
| 1,1,1-Trinitroethane             | lq             | -96.9                                      |                                            |                                                     |                                                       |
| Trinitroglycerol                 | lq             | -370.9                                     |                                            |                                                     |                                                       |
| Trinitromethane                  | lq             | -32.8                                      |                                            |                                                     |                                                       |
|                                  | g              | -0.2                                       |                                            |                                                     |                                                       |
| 2,4,6-Trinitrophenetole          | c              | -204.6                                     |                                            |                                                     |                                                       |
| 2,4,6-Trinitrophenol             | c              | -214.3                                     |                                            |                                                     |                                                       |
| 2,4,6-Trinitrophenylhydrazine    | c              | 36.8                                       |                                            |                                                     |                                                       |
| 2,4,6-Trinitrotoluene            | c              | -65.5                                      |                                            |                                                     |                                                       |
| 2,4,6-Trinitro-1,3-xylene        | c              | -102.5                                     |                                            |                                                     |                                                       |
| Trioctylamine                    | lq             | -584.9                                     |                                            |                                                     |                                                       |
| 1,3,6-Trioxacyclooctane          | lq             | -515.9                                     |                                            |                                                     |                                                       |
| 1,3,5-Trioxane                   | c              | -522.5                                     |                                            | 133.0                                               | 114.4                                                 |
| Triphenylamine                   | c              | 234.7                                      | 504.2                                      |                                                     |                                                       |
| Triphenylarsine                  | c              | 310.0                                      |                                            |                                                     |                                                       |
| Triphenylbismuthine              | c              | 469.0                                      |                                            |                                                     |                                                       |
| Triphenylborane                  | c              | 48.5                                       |                                            |                                                     |                                                       |
| Triphenylene                     | c              | 151.8                                      | 329.2                                      | 254.7                                               |                                                       |
| 1,1,1-Triphenylethane            | c              | 157.2                                      |                                            |                                                     |                                                       |
| 1,1,2-Triphenylethane            | c              | 130.2                                      |                                            |                                                     |                                                       |
| Triphenylethylene                | c              | 233.5                                      | 514.6                                      |                                                     |                                                       |
| 2,4,6-Triphenylimidazole         | c              | 272                                        |                                            |                                                     |                                                       |
| Triphenylmethane                 | c              | 171.2                                      | 412.5                                      | 312.1                                               | 295.0                                                 |
| Triphenylmethanol                | c              | -3.4                                       | 272.8                                      | 329.3                                               |                                                       |
| Triphenyl phosphate              | c              | -757                                       |                                            |                                                     |                                                       |
| Triphenylphosphine               | c              | 232.2                                      |                                            |                                                     |                                                       |
| Triphenylphosphine oxide         | c              | -60.3                                      |                                            |                                                     |                                                       |
| Triphenylstibine                 | c              | 329.3                                      |                                            |                                                     |                                                       |
| Tripropoxyborane                 | lq             | -1127.2                                    |                                            |                                                     |                                                       |
| Tripropylamine                   | lq             | -207.2                                     |                                            |                                                     |                                                       |
| Tripropynylamine                 | lq             | 814.2                                      |                                            |                                                     |                                                       |
| Tris(acetylacetonato)-chromium   | c              | -1533.0                                    |                                            |                                                     |                                                       |
| Tris(diethylamino)phosphine      | lq             | -289.5                                     |                                            |                                                     |                                                       |
| 1,1,1-Tris(hydroxymethyl)-ethane | c              | -744.6                                     |                                            |                                                     |                                                       |

**TABLE 6.1** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*Continued*)

| Substance                        | Physical State | $\Delta_f H^\circ$<br>kJ·mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ·mol <sup>-1</sup> | $S^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> | $C_p^\circ$<br>J·deg <sup>-1</sup> ·mol <sup>-1</sup> |
|----------------------------------|----------------|--------------------------------------------|--------------------------------------------|-----------------------------------------------------|-------------------------------------------------------|
| Tris(hydroxymethyl)nitro-methane | c              | - 735.6                                    |                                            |                                                     |                                                       |
| Tris(isopropoxy)borane           | lq             | - 293.3                                    |                                            |                                                     |                                                       |
| Tris(trimethylsilyl)amine        | c              | - 725.1                                    |                                            |                                                     |                                                       |
| (-)-Tryptophane                  | c              | - 415.3                                    | - 119.4                                    | 251.0                                               | 238.2                                                 |
| (-)-Tyrosine                     | c              | - 685.1                                    | - 385.7                                    | 214.0                                               | 216.4                                                 |
| Undecane                         | lq             | - 327.2                                    | 22.8                                       | 458.1                                               | 344.9                                                 |
| Undecanoic acid                  | c              | - 735.9                                    |                                            |                                                     |                                                       |
| 1-Undecanol                      | lq             | - 504.8                                    |                                            |                                                     |                                                       |
| 1-Undecene                       | g              | - 144.8                                    | 129.5                                      | 579.4                                               | 246.7                                                 |
| 10-Undecenoic acid               | c              | - 577                                      |                                            |                                                     |                                                       |
| Uracil                           | c              | - 429.4                                    |                                            |                                                     | 120.5                                                 |
| Urea                             | c              | - 333.1                                    | - 196.8                                    | 104.6                                               | 93.1                                                  |
|                                  | g              | - 245.8                                    |                                            |                                                     |                                                       |
| Urea nitrate                     | c              | - 564.0                                    |                                            |                                                     |                                                       |
| Urea oxalate                     | c              | - 1528.4                                   |                                            |                                                     |                                                       |
| 5-Ureidohydantoin                | c              | - 718.0                                    | - 434.0                                    | 195.1                                               |                                                       |
| Uric acid                        | c              | - 618.8                                    | - 358.8                                    | 173.2                                               | 166.1                                                 |
| (±)-Valine                       | c              | - 628.9                                    | - 359.0                                    | 178.9                                               | 168.8                                                 |
| Valylphenylalanine               | c              | - 767.8                                    |                                            |                                                     |                                                       |
| Vinyl acetate                    | g              | - 314.4                                    |                                            |                                                     |                                                       |
| Vinylbenzene                     | lq             | 103.8                                      |                                            |                                                     |                                                       |
| Vinylcyclohexane                 | lq             | - 88.7                                     |                                            |                                                     |                                                       |
| 4-Vinylcyclohexene               | lq             | 26.8                                       |                                            |                                                     |                                                       |
| Vinylcyclopentane                | lq             | - 34.8                                     |                                            |                                                     |                                                       |
| Vinylcyclopropane                | lq             | 122.5                                      |                                            |                                                     |                                                       |
| 2-Vinylpyridine                  | lq             | 157.1                                      |                                            |                                                     |                                                       |
| Xanthine                         | c              | - 379.6                                    | - 165.9                                    | 161.1                                               | 151.3                                                 |
| Xanthone                         | c              | - 191.5                                    |                                            |                                                     |                                                       |
| 1,2-Xylene                       | lq             | - 24.4                                     | 110.3                                      | 246.5                                               | 186.1                                                 |
|                                  | g              | 19.1                                       | 122.1                                      | 352.8                                               | 133.3                                                 |
| 1,3-Xylene                       | lq             | - 25.4                                     | 107.7                                      | 252.2                                               | 183.3                                                 |
|                                  | g              | 17.3                                       | 118.9                                      | 357.7                                               | 127.6                                                 |
| 1,4-Xylene                       | lq             | - 24.4                                     | 110.1                                      | 247.4                                               | 181.5                                                 |
|                                  | g              | 18.0                                       | 121.1                                      | 352.4                                               | 126.9                                                 |
| Xylitol                          | c              | - 1118.5                                   |                                            |                                                     |                                                       |
| D-(+)-Xylose                     | c              | - 1057.8                                   |                                            |                                                     |                                                       |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds*Abbreviations Used in the Table* $\Delta H_m$ , enthalpy of melting (at the melting point) in  $\text{kJ} \cdot \text{mol}^{-1}$  $\Delta H_v$ , enthalpy of vaporization (at the boiling point) in  $\text{kJ} \cdot \text{mol}^{-1}$  $\Delta H_s$ , enthalpy of sublimation (or vaporization at 298 K) in  $\text{kJ} \cdot \text{mol}^{-1}$  $C_p$ , specific heat (at temperature specified on the Kelvin scale) for the physical state in existence (or specified: c, lq, g) at that temperature in  $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  $\Delta H_t$ , enthalpy of transition (at temperature specified, superscript, measured in degrees Celsius) in  $\text{kJ} \cdot \text{mol}^{-1}$ 

| Substance                               | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$   |       |       |        |
|-----------------------------------------|--------------|--------------|--------------|---------|-------|-------|--------|
|                                         |              |              |              | 400 K   | 600 K | 800 K | 1000 K |
| Acenaphthene                            | 21.54        | 54.73        | 86.2         |         |       |       |        |
| Acenaphthylene                          |              |              | 73.0         |         |       |       |        |
| Acetaldehyde                            | 3.24         | 25.8         | 25.5         | 66.3(g) | 85.9  | 101.3 | 112.5  |
| Acetamide                               | 15.71        | 56.1         | 78.7         |         |       |       |        |
| Acetanilide                             |              | 64.7         | 80.8         |         |       |       |        |
| Acetic acid                             | 11.54        | 23.7         | 23.4         | 79.7    | 106.2 | 125.5 | 139.3  |
| Acetic anhydride                        | 10.5         | 38.2         | 48.3         | 129.1   | 174.1 | 204.6 | 226.4  |
| Acetone                                 | 5.69         | 29.1         | 31.0         | 92.1    | 122.8 | 144.9 | 162.0  |
| Acetonitrile, $\Delta H_t = 0.22^{-56}$ | 8.17         | 29.8         | 32.9         | 61.2    | 76.8  | 89.0  | 98.3   |
| Acetophenone                            |              | 38.8         | 55.9         |         |       |       |        |
| Acetyl bromide                          |              |              | 33.1         |         |       |       |        |
| Acetyl chloride                         |              |              | 30.1         | 78.9    | 97.0  | 110.0 | 119.7  |
| Acetylene                               | 3.8          | 17.0         | 21.3         | 50.1    | 58.1  | 63.5  | 68.0   |
| Acetylene- $d_2$                        |              |              |              | 54.8    | 61.9  | 67.4  | 71.8   |
| Acetylenedicarbonitrile                 |              |              | 28.8         | 94.8    | 106.2 | 114.1 | 119.8  |
| Acetyl fluoride                         |              |              | 25.1         |         |       |       |        |
| Acetyl iodide                           |              |              | 38.5         |         |       |       |        |
| Acrylic acid                            | 11.16        | 44.1         | 54.3         | 96.0    | 123.4 | 142.0 | 155.3  |
| Acrylonitrile                           | 6.23         | 32.6         | 33.5         | 76.8    | 96.7  | 110.6 | 120.8  |
| Adamantane                              |              |              | 59.7         |         |       |       |        |
| Adenine                                 |              |              | 108.8        |         |       |       |        |
| $\alpha$ -Alanine                       |              |              | 138.1        |         |       |       |        |
| Allyl <i>tert</i> -butyl sulfide        |              |              | 44.4         |         |       |       |        |
| Allyl ethyl sulfone                     |              |              | 83.7         |         |       |       |        |
| Allyl ethyl sulfoxide                   |              |              | 71.6         |         |       |       |        |
| Allyl methyl sulfone                    |              |              | 79.5         |         |       |       |        |
| Allyl trichloroacetate                  |              |              | 52.3         |         |       |       |        |
| 3-Aminoacetophenone                     | 12.1         |              |              |         |       |       |        |
| 4-Aminoacetophenone                     | 15.9         |              |              |         |       |       |        |
| 2-Aminobenzoic acid                     | 20.5         |              | 104.9        |         |       |       |        |
| 3-Aminobenzoic acid                     | 21.8         |              | 128.0        |         |       |       |        |
| 4-Aminobenzoic acid                     | 20.9         |              | 116.1        |         |       |       |        |
| 2-Aminoethanol                          | 20.5         | 50.9         |              |         |       |       |        |
| Aniline                                 | 10.56        | 42.4         | 55.8         | 143.0   | 192.8 | 225.1 | 230.9  |
| Anthracene                              | 28.83        | 56.5         | 101.5        |         |       |       |        |
| 9,10-Anthraquinone                      |              | 88.5         | 112.1        |         |       |       |        |
| <i>cis</i> -Azobenzene                  | 22.04        |              | 92.9         |         |       |       |        |
| <i>trans</i> -Azobenzene                | 22.6         | 93.8         |              |         |       |       |        |
| Azobutane                               |              |              | 49.3         |         |       |       |        |
| Azomethane                              |              |              |              | 93.9    | 123.1 | 145.7 | 162.6  |
| Azomethane- $d_6$                       |              |              |              | 110.7   | 142.8 | 165.2 | 180.6  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                              | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |       |       |        |
|--------------------------------------------------------|--------------|--------------|--------------|----------|-------|-------|--------|
|                                                        |              |              |              | 400 K    | 600 K | 800 K | 1000 K |
| Azoisopropane                                          |              |              | 36.0         |          |       |       |        |
| Azopropane                                             |              |              | 39.9         |          |       |       |        |
| <i>trans</i> -Azoxybenzene                             | 17.93        |              |              |          |       |       |        |
| Azulene                                                | 12.1         | 55.5         | 76.8         | 176.4    | 248.2 | 295.4 | 327.4  |
| Benzaldehyde                                           | 9.32         | 42.5         | 49.8         |          |       |       |        |
| Benzamide                                              | 18.49        |              |              |          |       |       |        |
| 1,2-Benzanthracene                                     |              |              | 123.0        |          |       |       |        |
| 2,3-Benzanthracene                                     |              |              | 126          |          |       |       |        |
| 1,2-Benzanthracene-9,10-dione                          |              |              | 82.8         |          |       |       |        |
| Benzene                                                | 9.95         | 30.7         | 33.8         | 113.5(g) | 160.1 | 190.5 | 211.4  |
| Benzenecetic acid                                      | 14.49        |              |              |          |       |       |        |
| 1,3-Benzenedicarboxylic acid                           |              |              | 106.7        |          |       |       |        |
| 1,4-Benzenedicarboxylic acid                           |              |              | 98.3         |          |       |       |        |
| Benzenethiol                                           | 11.48        | 39.9         | 47.6         |          |       |       |        |
| Benzil                                                 | 23.54        |              |              |          |       |       |        |
| Benzoic acid                                           | 18.06        | 50.6         | 91.1         | 138.4    | 196.7 | 234.9 | 260.7  |
| Benzoic anhydride                                      | 17.2         |              | 96.4         |          |       |       |        |
| Benzonitrile                                           | 10.88        | 45.9         | 52.5         | 140.8    | 187.4 | 217.9 | 238.8  |
| Benzo[ <i>def</i> ]phenanthrene                        | 17.1         |              | 100.2        |          |       |       |        |
| Benzophenone                                           | 18.19        |              | 94.1         |          |       |       |        |
| 1,4-Benzoquinone                                       | 18.53        |              | 62.8         |          |       |       |        |
| Benzo[ <i>f</i> ]quinoline                             |              |              | 83.1         |          |       |       |        |
| Benzo[ <i>h</i> ]quinoline                             |              |              | 80.8         |          |       |       |        |
| Benzo[ <i>b</i> ]thiophene, $\Delta H_t = 3.0^{-11.6}$ | 11.8         |              |              |          |       |       |        |
| Benzotrifluoride                                       |              |              | 37.6         |          |       |       |        |
| Benzoyl bromide                                        |              |              | 58.6         |          |       |       |        |
| Benzoyl chloride                                       |              |              | 54.8         |          |       |       |        |
| Benzoyl iodide                                         |              |              | 61.9         |          |       |       |        |
| 4-Benzphenanthrene                                     |              |              | 106.3        |          |       |       |        |
| Benzyl acetate                                         |              | 49.4         |              |          |       |       |        |
| Benzyl alcohol                                         | 8.97         | 50.5         | 60.3         |          |       |       |        |
| Benzylamine                                            |              |              | 60.2         |          |       |       |        |
| Benzyl benzoate                                        |              | 53.6         | 77.8         |          |       |       |        |
| Benzyl bromide                                         |              |              | 47.3         |          |       |       |        |
| Benzyl chloride                                        |              |              | 51.5         |          |       |       |        |
| Benzyl ethyl sulfide                                   |              |              | 56.9         |          |       |       |        |
| Benzyl iodide                                          |              |              | 47.3         |          |       |       |        |
| Benzyl mercaptan                                       |              |              | 56.6         |          |       |       |        |
| Benzyl methyl ketone                                   |              |              | 49.0         |          |       |       |        |
| Benzyl methyl sulfide                                  |              |              | 53.6         |          |       |       |        |
| Bicyclo[1.1.0]butane                                   |              |              | 23.4         |          |       |       |        |
| Bicyclo[2.2.1]hepta-2,5-dione                          |              | 32.9         |              |          |       |       |        |
| Bicyclo[2.2.1]heptane                                  |              |              | 40.2         |          |       |       |        |
| Bicyclo[4.1.0]heptane                                  |              |              | 38.0         |          |       |       |        |
| Bicyclo[2.2.1]-2-heptene                               |              |              | 38.8         |          |       |       |        |
| Bicyclo[3.1.0]hexane                                   |              |              | 32.8         |          |       |       |        |
| Bicyclohexyl                                           |              |              | 58.0         |          |       |       |        |
| Bicyclo[2.2.2]octane                                   |              |              | 48.0         |          |       |       |        |
| Bicyclo[4.2.0]octane                                   |              |              | 42.0         |          |       |       |        |
| Bicyclo[5.1.0]octane                                   |              |              | 43.5         |          |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                 | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|-------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                           |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Bicyclo[2.2.2]-2-octene                   |              |              | 43.8         |       |       |       |        |
| Bicyclopropyl                             |              |              | 33.5         |       |       |       |        |
| Biphenyl                                  | 18.6         | 45.6         | 81.8         | 221.0 | 307.7 | 363.7 | 401.7  |
| Biphenylene                               |              |              | 84.3         |       |       |       |        |
| Bis(2-butoxyethyl) ether                  |              | 55.9         |              |       |       |       |        |
| Bis(2-chloroethyl) ether                  | 8.66         | 45.2         |              |       |       |       |        |
| Bis(2-ethoxyethyl) ether                  |              | 49.0         |              |       |       |       |        |
| Bis(2-ethoxymethyl) ether                 |              | 36.2         | 44.7         |       |       |       |        |
| Bis(2-hydroxyethyl) ether                 |              | 52.3         | 57.3         |       |       |       |        |
| Bis(2-methoxyethyl) ether                 |              | 43.1         |              |       |       |       |        |
| Bromobenzene                              | 10.62        | 37.9         | 44.5         | 127.4 | 171.5 | 199.9 | 219.2  |
| 4-Bromobenzoic acid                       |              |              | 87.9         |       |       |       |        |
| 1-Bromobutane                             | 6.69         | 32.5         | 36.7         | 136.6 | 180.0 | 211.2 | 234.4  |
| (±)-2-Bromobutane                         | 6.89         | 30.8         | 34.4         | 138.1 | 214.7 | 238.2 |        |
| 1-Bromo-2-chloroethane                    |              | 33.7         | 38.2         |       |       |       |        |
| Bromochloromethane                        |              | 30.0         | 32.8         |       |       |       |        |
| 1-Bromo-3-chloropropane                   |              | 37.6         | 44.1         |       |       |       |        |
| 1-Bromo-2-chloro-1,1,2-trifluoroethane    |              | 28.3         | 30.1         |       |       |       |        |
| Bromochloro-2,2,2-trifluoroethane         |              | 28.1         | 29.8         |       |       |       |        |
| 1-Bromododecane                           |              | 74.8         |              |       |       |       |        |
| Bromoethane                               | 5.86         | 27.0         | 28.0         | 79.2  | 102.8 | 119.6 | 132.2  |
| Bromoethylene                             | 5.12         | 23.4         | 18.2         | 66.6  | 83.0  | 94.1  | 102.3  |
| 1-Bromoheptane                            |              |              | 50.6         |       |       | 74.8  |        |
| 1-Bromohexadecane                         |              |              | 94.4         |       |       |       |        |
| 1-Bromohexane                             |              |              | 45.9         |       |       |       |        |
| Bromomethane, $\Delta H_t = 0.47^{-99.4}$ | 5.98         | 23.9         | 22.8         | 50.0  | 62.7  | 72.2  | 79.5   |
| 1-Bromo-2-methylpropane                   |              | 31.3         | 34.8         |       |       |       |        |
| 2-Bromo-2-methylpropane                   | 1.97         | 29.2         | 31.8         | 146.1 | 190.7 | 220.3 | 241.6  |
| $\Delta H_t = 5.7^{-64.5}$                |              |              |              |       |       |       |        |
| $\Delta H_t = 1.0^{-41.6}$                |              |              |              |       |       |       |        |
| 1-Bromonaphthalene                        | 15.16        | 39.3         | 52.5         |       |       |       |        |
| 1-Bromooctane                             |              |              | 55.8         |       |       |       |        |
| 1-Bromopentane                            | 11.46        | 35.0         | 41.3         | 165.6 | 219.0 | 257.5 | 286.0  |
| 1-Bromopropane                            | 6.53         | 29.8         | 32.0         | 107.5 | 140.8 | 164.9 | 182.8  |
| 2-Bromopropane                            |              | 28.3         | 30.2         | 110.2 | 144.0 | 167.7 | 185.2  |
| 3-Bromopropene                            |              | 30.2         | 32.7         |       |       |       |        |
| Bromotrichloromethane                     | 2.54         |              |              |       |       |       |        |
| Bromotrifluoromethane                     |              |              |              | 79.3  | 91.3  | 97.5  | 100.9  |
| Bromotrimethylsilane                      |              |              | 32.6         |       |       |       |        |
| 1,2-Butadiene                             | 7.0          | 24.0         | 23.2         | 98.4  | 128.5 | 150.7 | 167.4  |
| 1,3-Butadiene                             | 7.98         | 22.5         | 20.9         | 101.2 | 154.1 | 169.5 |        |
| 1,3-Butadiyne                             |              |              |              | 84.4  | 96.8  | 105.1 | 111.3  |
| Butanal                                   | 11.09        | 31.5         | 34.5         | 126.4 | 165.7 | 195.0 | 216.3  |
| Butanamide                                | 17.6         |              | 85.9         |       |       |       |        |
| Butane, $\Delta H_t = 2.1^{-165.6}$       | 4.66         | 22.4         | 21.0         | 123.9 | 168.6 | 201.8 | 226.9  |
| 1,2-Butanediamine                         |              |              | 46.3         |       |       |       |        |
| Butanedinitrile                           | 3.7          | 48.5         | 70.0         |       |       |       |        |
| 1,3-Butanediol                            |              | 58.5         | 67.8         |       |       |       |        |
| 1,4-Butanediol                            |              |              | 76.6         |       |       |       |        |
| 2,3-Butanediol                            |              |              | 59.2         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                              | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                        |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 2,3-Butanedione                        |              |              | 38.7         |       |       |       |        |
| 1,4-Butanedithiol                      |              |              | 55.1         |       |       |       |        |
| Butanenitrile                          | 5.02         | 33.7         | 39.3         | 118.8 | 155.1 | 181.9 | 201.8  |
| <i>meso</i> -1,2,3,4-Butanetetrol      |              |              | 135.1        |       |       |       |        |
| 1,4-Butanedithiol                      |              |              | 49.7         |       |       |       |        |
| 1-Butanethiol                          | 10.46        | 32.2         | 36.6         | 146.2 | 194.7 | 233.0 | 263.4  |
| 2-Butanethiol                          | 6.5          | 30.6         | 34.0         | 148.0 | 194.2 | 227.2 | 251.1  |
| 1,2,4-Butanetriol                      |              |              | 58.6         |       |       |       |        |
| Butanoic acid                          | 11.08        | 41.8         | 40.5         |       |       |       |        |
| Butanoic anhydride                     |              | 50.0         |              |       |       |       |        |
| 1-Butanol                              | 9.28         | 43.3         | 52.3         | 137.2 | 183.7 | 218.0 | 243.8  |
| 2-Butanol                              |              | 40.8         | 49.7         | 141.0 | 187.1 | 220.4 | 245.3  |
| 2-Butanone                             | 8.44         | 31.3         | 34.8         | 124.7 | 163.6 | 192.8 | 214.8  |
| <i>trans</i> -2-Butenal                |              |              | 34.5         |       |       |       |        |
| 1-Butene                               | 3.9          | 22.1         | 20.2         | 109.0 | 147.1 | 174.9 | 195.9  |
| <i>cis</i> -2-Butene                   | 7.58         | 23.3         | 22.2         | 101.8 | 141.4 | 171.0 | 193.1  |
| <i>trans</i> -2-Butene                 | 9.8          | 22.7         | 21.4         | 108.9 | 145.6 | 184.9 | 194.9  |
| <i>cis</i> -2-Butenedinitrile          |              |              | 72.0         |       |       |       |        |
| <i>cis</i> -2-Butenedioic acid         |              |              | 110.0        |       |       |       |        |
| <i>trans</i> -2-Butenedioic acid       |              |              | 136.3        |       |       |       |        |
| <i>cis</i> -2-Butene-1,4-diol          |              | 66.1         |              |       |       |       |        |
| <i>trans</i> -2-Butene-1,4-diol        |              | 69.0         |              |       |       |       |        |
| <i>cis</i> -2-Butenenitrile            |              |              | 38.9         |       |       |       |        |
| <i>trans</i> -2-Butenenitrile          |              |              | 40.0         |       |       |       |        |
| 3-Butenenitrile                        |              |              | 40.0         |       |       |       |        |
| <i>cis</i> -2-Butenoic acid            | 12.57        |              |              |       |       |       |        |
| <i>trans</i> -2-Butenoic acid          | 12.98        |              |              |       |       |       |        |
| <i>cis</i> -2-Buten-1-ol               |              | 46.4         |              |       |       |       |        |
| 1-Buten-3-yne                          |              |              |              | 89.0  | 111.6 | 127.2 | 138.7  |
| 2-Butoxyethanol                        |              |              | 56.6         |       |       |       |        |
| 1- <i>tert</i> -Butoxy-2-ethoxyethane  |              |              | 50.9         |       |       |       |        |
| 2-(2-Butoxyethoxy)ethanol              |              | 28.0         |              |       |       |       |        |
| 2-Butoxyethyl acetate                  |              |              | 59.5         |       |       |       |        |
| 1- <i>tert</i> -Butoxy-2-methoxyethane |              | 38.5         | 47.8         |       |       |       |        |
| <i>N</i> -Butylacetamide               |              |              | 76.1         |       |       |       |        |
| Butyl acetate                          |              | 36.3         | 43.9         |       |       |       |        |
| <i>tert</i> -Butyl acetate             |              | 33.1         | 38.0         |       |       |       |        |
| Butylamine                             |              | 31.8         | 35.7         | 148.3 | 197.9 | 234.4 | 261.7  |
| <i>sec</i> -Butylamine                 |              | 29.9         | 32.8         | 148.1 | 199.0 | 236.1 | 261.7  |
| <i>tert</i> -Butylamine                | 0.88         | 28.3         | 29.6         | 152.6 | 204.5 | 240.5 | 266.9  |
| Butylbenzene                           | 11.22        | 38.9         | 51.4         | 229.1 | 314.6 | 373.9 | 416.3  |
| <i>sec</i> -Butylbenzene               | 9.83         | 38.0         | 48.0         |       |       |       |        |
| <i>tert</i> -Butylbenzene              | 8.39         | 37.6         | 47.7         |       |       |       |        |
| <i>sec</i> -Butyl butanoate            |              |              | 47.3         |       |       |       |        |
| Butyl chloroacetate                    |              |              | 51.0         |       |       |       |        |
| Butyl 2-chlorobutanoate                |              |              | 52.7         |       |       |       |        |
| Butyl 3-chlorobutanoate                |              |              | 53.1         |       |       |       |        |
| Butyl 4-chlorobutanoate                |              |              | 54.4         |       |       |       |        |
| Butyl 2-chloropropanoate               |              |              | 54.4         |       |       |       |        |
| Butyl 3-chlorobutanoate                |              |              | 55.4         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                     | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|-------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                               |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Butyl crotonate               |              |              | 51.9         |       |       |       |        |
| sec-Butyl crotonate           |              |              | 49.4         |       |       |       |        |
| Butylcyclohexane              | 14.16        | 38.5         | 49.4         | 276.1 | 289.5 | 469.9 | 525.9  |
| Butylcyclopentane             | 11.3         | 36.2         | 45.9         | 241.7 | 336.3 | 407.3 | 480.3  |
| N-Butyldiacetamide            |              |              | 64.4         |       |       |       |        |
| Butyl dichloroacetate         |              |              | 52.3         |       |       |       |        |
| Butylethylamine               |              | 34.0         | 40.2         |       |       |       |        |
| Butyl ethyl ether             |              | 31.6         | 36.3         |       |       |       |        |
| Butyl ethyl sulfide           | 12.4         | 37.0         | 44.5         | 202.4 | 271.8 | 325.3 | 367.2  |
| tert-Butyl ethyl sulfide      | 7.1          | 33.5         | 39.3         |       |       |       |        |
| Butyl formate                 |              | 36.6         | 41.1         |       |       |       |        |
| tert-Butyl hydroperoxide      |              |              | 47.7         |       |       |       |        |
| Butylisopropylamine           |              | 34.5         | 42.1         |       |       |       |        |
| Butyllithium                  |              |              | 107.1        |       |       |       |        |
| Butyl methyl ether            |              | 29.6         | 32.4         |       |       |       |        |
| sec-Butyl methyl ether        |              | 28.1         | 30.2         |       |       |       |        |
| tert-Butyl methyl ether       |              | 27.9         | 29.8         |       |       |       |        |
| Butyl methyl sulfide          | 12.5         | 34.5         | 40.5         | 174.6 | 233.0 | 278.4 | 314.1  |
| tert-Butyl methyl sulfide     | 8.4          | 31.5         | 35.8         |       |       |       |        |
| Butyl methyl sulfone          |              |              | 76.2         |       |       |       |        |
| tert-Butyl methyl sulfone     |              |              | 82.4         |       |       |       |        |
| Butyl octadecanoate           | 56.90        |              |              |       |       |       |        |
| tert-Butyl peroxide           |              |              | 31.8         |       |       |       |        |
| Butyl propyl ether            |              | 33.7         | 40.2         |       |       |       |        |
| Butyl thiolacetate            |              |              | 48.1         |       |       |       |        |
| Butyl trichloroacetate        |              |              | 53.6         |       |       |       |        |
| Butyl vinyl ether             |              | 31.6         | 36.2         |       |       |       |        |
| 1-Butyne                      | 6.0          | 24.5         | 23.3         | 99.9  | 129.0 | 150.4 | 166.7  |
| 2-Butyne                      | 9.23         | 26.5         | 26.6         | 94.6  | 124.2 | 147.0 | 164.4  |
| 2-Butynedinitrile             |              |              | 28.8         |       |       |       |        |
| 4-Butyrolactone               | 9.57         | 52.2         |              |       |       |       |        |
| Butyrophenone                 |              |              | 60.7         |       |       |       |        |
| (+)-Camphor                   | 6.84         | 59.5         |              |       |       |       |        |
| 9H-Carbazole                  | 26.9         |              | 84.5         |       |       |       |        |
| Chloroacetic acid             | 12.28        |              | 75.3         |       |       |       |        |
| Chloroacetyl chloride         |              |              | 38.9         |       |       |       |        |
| 2-Chloroaniline               | 11.88        | 44.4         | 56.8         |       |       |       |        |
| 2-Chlorobenzaldehyde          |              |              | 53.1         |       |       |       |        |
| Chlorobenzene                 | 9.61         | 35.2         | 41.0         | 128.1 | 172.2 | 200.4 | 219.6  |
| 2-Chlorobenzoic acid          | 25.73        |              | 79.5         |       |       |       |        |
| 3-Chlorobenzoic acid          |              |              | 82.0         |       |       |       |        |
| 4-Chlorobenzoic acid          |              |              | 87.9         |       |       |       |        |
| Chloro-1,4-benzoquinone       |              |              | 69.0         |       |       |       |        |
| 1-Chlorobutane                |              | 30.4         | 33.5         | 135.1 | 179.0 | 210.5 | 234.0  |
| 2-Chlorobutane                |              | 29.2         | 31.5         | 136.1 | 180.7 | 212.7 | 236.8  |
| Chlorocyclohexane             |              |              | 43.5         |       |       |       |        |
| 1-Chloro-1,1-difluoroethane   | 2.69         | 22.4         |              |       |       |       |        |
| Chlorodifluoromethane         | 4.12         | 20.2         |              | 65.4  | 78.9  | 87.2  | 92.4   |
| 2-Chloro-1,4-dihydroxybenzene |              |              | 69.0         |       |       |       |        |
| Chlorodimethylsilane          |              | 26.2         |              |       |       |       |        |



**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$   |       |       |        |
|------------------------------------------|--------------|--------------|--------------|---------|-------|-------|--------|
|                                          |              |              |              | 400 K   | 600 K | 800 K | 1000 K |
| Chlorodiphenylsilane                     |              |              | 69.5         |         |       |       |        |
| 1-Chloro-2,3-epoxypropane                |              | 33.1         | 40.6         |         |       |       |        |
| Chloroethane                             | 4.45         | 24.7         |              | 77.6    | 101.6 | 118.8 | 131.7  |
| 2-Chloroethanol                          |              | 41.4         |              |         |       |       |        |
| 1-Chloro-2-ethylbenzene                  |              |              | 47.3         |         |       |       |        |
| 1-Chloro-4-ethylbenzene                  |              |              | 48.1         |         |       |       |        |
| Chloroethylene                           | 4.75         | 20.8         |              | 65.0    | 82.1  | 93.5  | 101.9  |
| 2-Chloroethyl vinyl ether                |              | 38.2         |              |         |       |       |        |
| Chloroethyne                             |              |              |              | 60.2    | 66.8  | 71.0  | 74.3   |
| 1-Chloroheptane                          |              |              | 47.7         |         |       |       |        |
| 1-Chlorohexane                           |              | 35.7         | 42.8         |         |       |       |        |
| Chlorohydroquinone                       |              |              | 69.0         |         |       |       |        |
| Chloromethane                            | 6.43         | 21.4         | 18.9         | 48.2    | 61.3  | 71.3  | 78.9   |
| 1-Chloro-2-methylbenzene                 | 8.37         | 37.5         |              |         |       |       |        |
| 1-Chloro-3-methylbenzene                 | 10.46        |              |              |         |       |       |        |
| 1-Chloro-4-methylbenzene                 |              | 38.7         |              |         |       |       |        |
| 1-Chloro-3-methylbutane                  |              | 32.0         | 36.2         |         |       |       |        |
| 1-Chloro-2-methylpropane                 |              | 29.2         | 31.7         | 136.1   | 180.7 | 212.7 | 236.8  |
| 2-Chloro-2-methylpropane                 | 2.09         | 27.6         | 29.0         | 142.3   | 184.9 | 215.5 | 238.5  |
| $\Delta H_t = 1.7^{-90.1}$               |              |              |              |         |       |       |        |
| $\Delta H_t = 5.8^{-53.6}$               |              |              |              |         |       |       |        |
| 1-Chloronaphthalene                      | 12.90        | 52.1         | 65.3         |         |       |       |        |
| 2-Chloronaphthalene                      |              |              | 82.0         |         |       |       |        |
| 1-Chloro-3-nitrobenzene                  | 19.37        |              |              |         |       |       |        |
| 1-Chloro-4-nitrobenzene                  | 20.77        |              |              |         |       |       |        |
| 1-Chlorooctane                           |              |              | 52.4         |         |       |       |        |
| Chloropentafluoroacetone                 |              |              | 25.3         |         |       |       |        |
| Chloropentafluorobenzene                 |              | 34.8         | 41.1         |         |       |       |        |
| Chloropentafluoroethane                  | 1.88         | 19.4         |              |         |       |       |        |
| 1-Chloropentane                          |              | 33.2         | 38.2         | 164.2   | 218.0 | 256.8 | 285.6  |
| 2-Chloropentane                          |              | 31.8         | 36.0         |         |       |       |        |
| 2-Chlorophenol                           | 12.52        |              |              |         |       |       |        |
| 3-Chlorophenol                           | 14.91        |              | 53.1         |         |       |       |        |
| 4-Chlorophenol                           | 14.07        |              | 51.9         |         |       |       |        |
| 1-Chloropropane                          | 5.54         | 27.2         | 28.4         | 106.1   | 139.9 | 164.2 | 182.4  |
| 2-Chloropropane                          | 7.39         | 26.3         | 26.9         | 108.7   | 143.1 | 167.1 | 184.8  |
| 3-Chloro-1-propene                       |              | 29.0         | 28.2         | 92.6    | 111.0 | 137.8 | 151.9  |
| Chlorotrifluoroethylene                  | 5.6          | 20.8         |              |         |       |       |        |
| Chlorotrifluoromethane                   |              | 15.8         |              | 77.5    | 90.3  | 96.9  | 100.5  |
| Chlorotrimethylsilane                    |              | 27.6         | 30.1         |         |       |       |        |
| Chlorotrinitromethane                    |              |              | 45.4         |         |       |       |        |
| Chrysene                                 | 26.15        |              | 124.5        |         |       |       |        |
| Coronene                                 | 19.2         |              |              |         |       |       |        |
| 1,2-Cresol                               | 13.94        | 45.2         | 76.0         | 166.3   | 220.8 | 257.5 | 287.9  |
| 1,3-Cresol                               | 9.41         | 47.4         | 61.7         | 162.1   | 218.7 | 256.4 | 286.6  |
| 1,4-Cresol                               | 11.89        | 47.5         | 73.9         | 161.7   | 218.0 | 255.7 | 286.5  |
| Cubane                                   |              |              | 80.3         |         |       |       |        |
| Cyanamide                                | 8.76         | 68.6         |              |         |       |       |        |
| Cyanogen                                 | 8.1          | 23.3         | 19.7         | 61.9(g) | 68.2  | 72.9  | 76.4   |
| Cyclobutane, $\Delta H_t = 5.8^{-126.8}$ | 1.1          | 24.2         | 23.5         | 100.0   | 145.4 | 177.5 | 200.7  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                   | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|-----------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                             |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Cyclobutanecarbonitrile     |              | 36.9         | 44.3         |       |       |       |        |
| Cyclobutanenitrile          |              |              | 40.0         |       |       |       |        |
| Cyclobutene                 |              |              |              | 90.3  | 126.8 | 151.7 | 169.6  |
| Cyclobutylamine             |              |              | 35.6         |       |       |       |        |
| Cyclododecane               |              |              | 76.4         |       |       |       |        |
| Cycloheptane                | 1.88         | 33.2         | 38.5         | 175.0 | 261.2 | 322.3 | 365.7  |
| $\Delta H_t = 5.0^{-138.4}$ |              |              |              |       |       |       |        |
| $\Delta H_t = 0.3^{-75.0}$  |              |              |              |       |       |       |        |
| $\Delta H_t = 0.5^{-60.8}$  |              |              |              |       |       |       |        |
| Cycloheptanone              |              |              | 51.9         |       |       |       |        |
| 1,3,5-Cycloheptatriene      | 1.2          | 38.7         |              | 155.4 | 209.5 | 245.1 | 270.2  |
| $\Delta H_t = 2.4^{-119.2}$ |              |              |              |       |       |       |        |
| Cyclohexane                 | 2.63         | 30.0         | 33.0         | 149.9 | 225.2 | 279.3 | 317.2  |
| $\Delta H_t = 6.7^{-87}$    |              |              |              |       |       |       |        |
| Cyclohexanecarbonitrile     |              |              | 51.9         |       |       |       |        |
| Cyclohexanethiol            |              | 37.1         | 44.6         |       |       |       |        |
| Cyclohexanol                | 1.76         | 45.5         | 62.0         | 172.1 | 248.1 | 302.0 | 339.5  |
| $\Delta H_t = 8.2^{-9.7}$   |              |              |              |       |       |       |        |
| Cyclohexanone               |              | 40.3         | 45.1         | 150.6 | 221.3 | 272.0 | 305.4  |
| Cyclohexene                 | 3.29         | 30.5         | 33.5         | 144.9 | 206.9 | 248.9 | 278.7  |
| $\Delta H_t = 4.3^{-134.4}$ |              |              |              |       |       |       |        |
| 1-Cyclohexenecarbonitrile   |              |              | 53.5         |       |       |       |        |
| Cyclohexylamine             |              | 36.1         | 43.7         |       |       |       |        |
| Cyclohexylbenzene           | 15.30        |              | 59.9         |       |       |       |        |
| Cyclohexylcyclohexane       |              | 51.9         | 58.0         |       |       |       |        |
| cis, cis-1,5-Cyclooctadiene |              |              | 43.4         |       |       |       |        |
| Cyclooctane                 | 2.41         | 35.9         | 43.3         | 200.1 | 297.1 | 365.3 | 414.3  |
| $\Delta H_t = 6.3^{-106.7}$ |              |              |              |       |       |       |        |
| $\Delta H_t = 0.5^{-89.4}$  |              |              |              |       |       |       |        |
| Cyclooctanone               |              |              | 54.4         |       |       |       |        |
| 1,3,5,7-Cyclooctatetraene   | 11.3         | 36.4         | 43.1         | 160.9 | 220.8 | 260.4 | 288.2  |
| Cyclooctene                 |              |              | 47.0         |       |       |       |        |
| Cyclopentadiene             |              |              | 28.4         |       |       |       |        |
| Cyclopentane                | 0.61         | 27.3         | 28.5         | 118.7 | 178.1 | 220.1 | 250.4  |
| $\Delta H_t = 4.8^{-150.8}$ |              |              |              |       |       |       |        |
| $\Delta H_t = 0.3^{-135.1}$ |              |              |              |       |       |       |        |
| Cyclopentanecarbonitrile    |              |              | 43.4         |       |       |       |        |
| 1-Cyclopentenecarbonitrile  |              |              | 45.0         |       |       |       |        |
| Cyclopentanethiol           | 7.8          | 35.3         | 41.4         | 144.5 | 203.6 | 245.2 | 275.5  |
| Cyclopentanol               |              |              | 57.6         |       |       |       |        |
| Cyclopentanone              |              | 36.4         | 42.7         |       |       |       |        |
| Cyclopentene                | 3.36         |              | 28.1         | 104.9 | 155.6 | 191.5 | 217.3  |
| $\Delta H_t = 0.5^{-186.1}$ |              |              |              |       |       |       |        |
| Cyclopentylamine            | 8.31         |              | 40.2         |       |       |       |        |
| Cyclopropane                | 5.44         | 20.1         | 16.9         | 76.6  | 109.4 | 140.5 | 148.1  |
| Cyclopropanecarbonitrile    |              | 35.6         | 41.9         |       |       |       |        |
| Cyclopropylamine            | 13.18        |              | 31.3         |       |       |       |        |
| Cyclopropylbenzene          |              |              | 50.2         |       |       |       |        |
| Cyclopropyl methyl ketone   |              | 34.1         | 38.4         |       |       |       |        |
| Decafluorobutane            |              | 22.9         |              |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                                      | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                                |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| <i>cis</i> -Decahydronaphthalene<br>$\Delta H_t = 2.1^{-57.1}$ | 9.49         | 41.0         | 50.2         | 237.0 | 352.0 | 432.5 | 489.5  |
| <i>trans</i> -Decahydronaphthalene                             | 14.41        | 40.2         | 43.5         | 237.6 | 352.3 | 432.6 | 489.2  |
| Decanal                                                        |              |              |              | 300.4 | 400.4 | 472.8 | 525.9  |
| Decane                                                         | 28.78        | 38.8         |              | 298.1 | 403.2 | 480.8 | 536.4  |
| Decanedioic acid                                               | 40.8         |              | 160.7        |       |       |       |        |
| Decanenitrile                                                  |              |              | 66.8         |       |       |       |        |
| 1-Decanethiol                                                  | 31.0         | 46.4         | 65.5         | 320.6 | 429.4 | 510.9 | 573.1  |
| Decanoic acid                                                  | 28.02        |              | 118.8        |       |       |       |        |
| 1-Decanol                                                      | 37.7         | 49.8         | 81.5         | 187.2 | 418.2 | 495.9 | 553.3  |
| 1-Decene                                                       | 21.10        | 38.7         | 50.4         | 283.6 | 381.9 | 453.0 | 505.9  |
| $\Delta H_t = 8.0^{-74.8}$                                     |              |              |              |       |       |       |        |
| 1-Decyne                                                       |              |              |              | 274.6 | 363.8 | 428.5 | 476.6  |
| Deoxybenzoin                                                   |              |              | 93.3         |       |       |       |        |
| Dibenz[ <i>de,kl</i> ]anthracene                               |              |              | 125.5        |       |       |       |        |
| Dibenzoyl peroxide                                             | 31.4         |              | 102.5        |       |       |       |        |
| Dibenzyl ether                                                 |              | 20.2         |              |       |       |       |        |
| Dibenzyl sulfide                                               |              |              | 93.3         |       |       |       |        |
| Dibenzyl sulfone                                               |              |              | 125.5        |       |       |       |        |
| 1,2-Dibromobutane                                              |              |              | 50.3         | 153.9 | 195.4 | 224.3 | 244.8  |
| 1,4-Dibromobutane                                              |              |              | 53.1         |       |       |       |        |
| 2,3-Dibromobutane                                              |              |              | 37.7         |       |       |       |        |
| 1,2-Dibromo-1-chloro-1,1,2-trifluoroethane                     |              | 31.2         | 35.0         |       |       |       |        |
| 1,2-Dibromocycloheptane                                        |              |              | 52.0         |       |       |       |        |
| 1,2-Dibromocyclohexane                                         |              |              | 50.5         |       |       |       |        |
| 1,2-Dibromocyclooctane                                         |              |              | 54.6         |       |       |       |        |
| 1,2-Dibromoethane                                              | 10.84        | 34.8         | 41.7         | 99.7  | 122.3 | 137.8 | 149.8  |
| 1,2-Dibromoheptane                                             |              |              | 54.4         |       |       |       |        |
| Dibromomethane                                                 |              | 32.9         | 37.0         | 63.0  | 74.8  | 82.5  | 88.0   |
| 1,2-Dibromopropane                                             | 8.94         | 35.6         | 41.7         | 124.4 | 157.4 | 179.5 | 195.6  |
| 1,3-Dibromopropane                                             | 13.6         |              | 47.5         |       |       |       |        |
| 1,2-Dibromotetrafluoroethane                                   | 7.04         | 27.0         | 28.4         |       |       |       |        |
| 1,2-Dibutoxyethane                                             |              | 47.8         | 58.8         |       |       |       |        |
| Dibutoxymethane                                                |              |              | 48.1         |       |       |       |        |
| Dibutylamine                                                   |              | 38.4         | 49.5         |       |       |       |        |
| <i>N,N</i> -Dibutyl-1-butanamine                               |              | 46.9         |              |       |       |       |        |
| Dibutyl decanedioate                                           |              | 92.9         |              |       |       |       |        |
| Dibutyl disulfide                                              |              | 46.9         | 64.5         | 286.1 | 376.5 | 442.8 | 493.1  |
| Di- <i>tert</i> -butyl disulfide                               |              |              | 54.3         |       |       |       |        |
| Dibutyl ether                                                  |              | 36.5         | 45.0         | 254.3 | 340.1 | 403.8 | 451.3  |
| Di- <i>sec</i> -butyl ether                                    |              | 34.1         | 40.8         |       |       |       |        |
| Di- <i>tert</i> -butyl ether                                   |              | 32.2         | 37.6         |       |       |       |        |
| Dibutylmercury                                                 |              |              | 63.5         |       |       |       |        |
| Di- <i>tert</i> -butyl peroxide                                |              |              | 31.8         |       |       |       |        |
| Dibutyl 1,2-phthalate                                          |              | 79.2         | 91.6         |       |       |       |        |
| Dibutyl sulfate                                                |              |              | 75.9         |       |       |       |        |
| Dibutyl sulfide                                                | 19.4         | 41.3         | 53.0         | 259.8 | 348.6 | 420.8 | 475.8  |
| Di- <i>tert</i> -butyl sulfide                                 |              | 33.3         | 43.8         |       |       |       |        |
| Dibutyl sulfite                                                |              |              | 67.8         |       |       |       |        |
| Dibutyl sulfone                                                |              |              | 100.4        |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                          | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                    |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Dichloroacetyl chloride            |              |              | 39.3         |       |       |       |        |
| 1,2-Dichlorobenzene                | 12.93        | 39.7         | 50.2         | 142.8 | 184.4 | 210.4 | 227.7  |
| 1,3-Dichlorobenzene                | 12.64        | 38.6         | 48.6         | 143.0 | 184.5 | 210.4 | 227.7  |
| 1,4-Dichlorobenzene                | 17.15        | 38.8         | 49.0         | 143.3 | 184.8 | 210.7 | 227.9  |
| 2,6-Dichlorobenzoquinone           |              |              | 69.9         |       |       |       |        |
| 2,2'-Dichlorobiphenyl              |              |              | 96.2         |       |       |       |        |
| 4,4'-Dichlorobiphenyl              |              |              | 103.8        |       |       |       |        |
| 1,2-Dichlorobutane                 |              | 33.9         | 39.6         |       |       |       |        |
| 1,4-Dichlorobutane                 |              |              | 46.4         |       |       |       |        |
| Dichlorodifluoromethane            | 4.14         | 20.1         |              | 82.4  | 93.6  | 99.1  | 100.0  |
| Dichlorodimethylsilane             |              |              | 34.3         |       |       |       |        |
| Dichlorodiphenylsilane             |              |              | 69.5         |       |       |       |        |
| 1,1-Dichloroethane                 | 8.84         | 28.9         | 30.6         | 91.4  | 113.7 | 128.8 | 139.8  |
| 1,2-Dichloroethane                 | 8.83         | 32.0         | 35.2         | 92.1  | 112.6 | 127.2 | 138.1  |
| 1,1-Dichloroethylene               | 6.51         | 26.1         | 26.5         | 78.7  | 93.9  | 103.4 | 110.0  |
| <i>cis</i> -1,2-Dichloroethylene   | 7.20         | 30.2         | 31.0         | 77.0  | 93.0  | 102.9 | 109.8  |
| <i>trans</i> -1,2-Dichloroethylene | 11.98        | 28.9         | 29.3         | 77.7  | 93.2  | 102.9 | 109.8  |
| 2,2-Dichloroethyl ether            |              | 38.4         |              |       |       |       |        |
| Dichlorofluoromethane              |              | 25.2         |              | 70.2  | 82.4  | 89.6  | 94.2   |
| 1,2-Dichlorohexafluoropropane      |              | 26.3         | 26.9         |       |       |       |        |
| 1,2-Dichlorohexane                 |              |              | 48.2         |       |       |       |        |
| Dichloromethane                    | 6.00         | 28.1         | 28.8         | 59.6  | 72.4  | 80.8  | 86.8   |
| 1,2-Dichloro-4-methylbenzene       | 10.68        |              |              |       |       |       |        |
| 1,2-Dichloropentane                |              | 36.5         | 43.9         |       |       |       |        |
| 1,5-Dichloropentane                |              |              | 50.7         |       |       |       |        |
| ( $\pm$ )-1,2-Dichloropropane      | 6.40         | 31.8         | 36.0         | 119.7 | 152.6 | 175.6 | 192.8  |
| 1,3-Dichloropropane                |              | 35.2         | 40.8         | 120.0 | 151.5 | 173.9 | 190.4  |
| 2,2-Dichloropropane                |              | 29.3         | 32.6         | 127.9 | 159.2 | 179.9 | 194.8  |
| 1,3-Dichloro-2-propanol            |              |              | 66.9         |       |       |       |        |
| 1,2-Dichlorotetrafluoroethane      | 6.32         | 23.3         |              |       |       |       |        |
| Dicyanoacetylene                   |              |              | 28.8         |       |       |       |        |
| Dicyclopentadienyliron             |              |              | 73.6         |       |       |       |        |
| Dicyclopropyl ketone               |              |              | 53.7         |       |       |       |        |
| Diethanolamine                     | 25.10        | 65.2         |              |       |       |       |        |
| 1,1-Diethoxyethane                 |              | 36.3         | 43.2         |       |       |       |        |
| 1,2-Diethoxyethane                 |              | 36.3         | 43.2         |       |       |       |        |
| Diethoxymethane                    |              | 31.3         | 35.7         |       |       |       |        |
| 1,3-Diethoxypropane                |              | 37.2         | 45.9         |       |       |       |        |
| 2,2-Diethoxypropane                |              |              | 31.8         |       |       |       |        |
| Diethylamine                       |              | 29.1         | 31.3         | 143.9 | 197.2 | 235.0 | 263.2  |
| 1,2-Diethylbenzene                 | 16.8         | 39.4         | 52.8         | 234.4 | 316.6 | 374.6 | 416.3  |
| 1,3-Diethylbenzene                 | 11.0         | 39.4         | 52.5         | 230.2 | 314.6 | 379.7 | 415.8  |
| 1,4-Diethylbenzene                 | 10.6         | 39.4         | 52.5         | 228.8 | 313.1 | 372.5 | 414.9  |
| Diethyl carbonate                  |              | 36.2         | 43.6         |       |       |       |        |
| Diethyl disulfide                  | 9.4          | 37.6         | 45.2         | 171.1 | 218.6 | 251.8 | 276.0  |
| Diethylene glycol diethyl ether    | 13.60        | 49.0         | 58.4         |       |       |       |        |
| Diethylene glycol dimethyl ether   |              | 36.2         | 44.7         |       |       |       |        |
| Diethylene glycol monoethyl ether  |              | 47.5         |              |       |       |       |        |
| Diethylene glycol monomethyl ether |              | 46.6         |              |       |       |       |        |
| Diethyl ether                      | 7.27         | 26.5         | 27.1         | 138.1 | 183.8 | 218.7 | 244.8  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                          |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Diethyl malonate                         |              | 54.8         |              |       |       |       |        |
| Diethyl oxalate                          |              | 42.0         | 63.5         |       |       |       |        |
| Diethyl peroxide                         |              |              | 30.5         |       |       |       |        |
| 3,3-Diethylpentane                       | 10.09        | 34.6         | 42.0         |       |       |       |        |
| Diethyl 1,2-phthalate                    |              |              | 88.3         |       |       |       |        |
| Diethyl sulfide                          | 11.90        | 31.8         | 35.8         | 145.0 | 192.9 | 229.7 | 258.5  |
| Diethyl sulfite                          |              |              | 48.5         |       |       |       |        |
| Diethyl sulfone                          |              |              | 86.2         |       |       |       |        |
| Diethyl sulfoxide                        |              |              | 62.3         |       |       |       |        |
| Diethylzinc                              |              |              | 40.2         |       |       |       |        |
| 1,2-Difluorobenzene                      | 11.1         | 32.2         | 36.2         | 137.1 | 181.3 | 209.7 | 229.0  |
| 1,3-Difluorobenzene                      | 8.58         | 31.1         | 34.6         | 137.0 | 180.5 | 207.8 | 225.6  |
| 1,4-Difluorobenzene                      |              | 31.8         | 35.5         | 137.4 | 180.1 | 207.8 | 225.7  |
| 2,2'-Difluorobiphenyl                    |              |              | 95.0         |       |       |       |        |
| 4,4'-Difluorobiphenyl                    |              |              | 91.2         |       |       |       |        |
| 1,1-Difluoroethane                       |              | 21.6         | 19.1         | 83.4  | 107.5 | 124.3 | 136.3  |
| 1,1-Difluoroethylene                     |              |              |              | 71.8  | 89.2  | 100.2 | 107.7  |
| Difluoromethane                          |              |              |              | 51.1  | 65.8  | 76.2  | 83.7   |
| 9,10-Dihydroanthracene                   |              |              | 93.3         |       |       |       |        |
| Dihydro-2 <i>H</i> -pyran                |              |              | 32.2         |       |       |       |        |
| 5,12-Dihydrotetracene                    |              |              | 115.9        |       |       |       |        |
| 2,3-Dihydrothiophene                     |              | 33.2         | 37.7         |       |       |       |        |
| 2,5-Dihydrothiophene                     |              | 34.8         | 40.0         |       |       |       |        |
| 2,4-Dihydrothiophene-1,1-dioxide         |              |              | 62.8         |       |       |       |        |
| 1,4-Dihydroxybenzene                     | 27.11        |              | 99.2         |       |       |       |        |
| 1,2-Diiodobenzene                        |              |              | 64.9         |       |       |       |        |
| 1,2-Diiodoethane                         |              |              | 65.7         | 96.0  | 116.8 | 131.3 | 141.6  |
| Diiodomethane                            | 44.80        | 42.5         | 51.0         | 65.9  | 76.9  | 83.9  | 89.1   |
| Diisobutylamine                          |              |              | 39.3         |       |       |       |        |
| Diisobutyl ether                         |              | 34.0         | 40.9         |       |       |       |        |
| Diisobutyl sulfide                       |              |              | 48.7         |       |       |       |        |
| Diisopropylamine                         |              | 30.4         | 34.6         |       |       |       |        |
| Diisopropyl ether                        | 11.03        | 29.1         | 32.1         | 196.2 | 262.0 | 311.3 | 348.0  |
| Diisopropylmercury                       |              |              | 53.6         |       |       |       |        |
| Diisopropyl sulfide                      | 10.4         | 33.8         | 39.6         | 211.9 | 277.1 | 322.7 | 356.6  |
| Diketene                                 |              | 36.8         | 42.9         |       |       |       |        |
| 1,2-Dimethoxybenzene                     | 16.04        | 48.2         | 66.9         |       |       |       |        |
| 1,1-Dimethoxyethane                      |              |              | 30.5         |       |       |       |        |
| 1,2-Dimethoxyethane                      | 12.60        | 32.4         | 36.4         |       |       |       |        |
| Dimethoxymethane                         | 8.33         |              | 35.1         |       |       |       |        |
| 2,2-Dimethoxypropane                     |              |              | 29.4         |       |       |       |        |
| <i>N,N</i> -Dimethylacetamide            | 10.42        | 43.4         | 50.2         |       |       |       |        |
| Dimethylamine                            | 5.94         | 26.4         | 25.0         | 87.4  | 118.9 | 142.0 | 159.8  |
| Dimethylaminomethanol                    |              |              | 50.2         |       |       |       |        |
| <i>N,N</i> -Dimethylaminotrimethylsilane |              |              | 31.8         |       |       |       |        |
| <i>N,N</i> -Dimethylaniline              |              |              | 52.8         |       |       |       |        |
| 1,4-Dimethylbicyclo[2.2.1]heptane        |              | 33.3         | 38.9         |       |       |       |        |
| 2,3-Dimethylbicyclo[2.2.1]-2-heptene     |              | 34.9         | 42.2         |       |       |       |        |
| 2,2-Dimethylbutane                       | 0.58         | 26.3         | 27.7         | 182.8 | 251.0 | 298.7 | 333.5  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                                                                                       | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|-----------------------------------------------------------------------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                                                                                 |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| $\Delta H_f = 5.4^{-147.3}$<br>$\Delta H_f = 0.3^{-132.3}$<br>2,3-Dimethylbutane<br>$\Delta H_f = 6.5^{-137.1}$ | 0.80         | 27.4         | 29.1         | 181.2 | 247.7 | 314.6 | 331.0  |
| 2,2-Dimethyl-1-butanol                                                                                          |              | 42.6         | 56.1         |       |       |       |        |
| 2,3-Dimethyl-1-butanol                                                                                          |              | 47.3         |              |       |       |       |        |
| 3,3-Dimethyl-1-butanol                                                                                          |              | 46.4         |              |       |       |       |        |
| 2,3-Dimethyl-2-butanol                                                                                          |              | 40.4         | 51.0         |       |       |       |        |
| ( $\pm$ )-3,3-Dimethyl-2-butanol                                                                                |              | 43.9         |              |       |       |       |        |
| 3,3-Dimethyl-2-butanone                                                                                         |              | 33.4         | 37.9         |       |       |       |        |
| 2,3-Dimethyl-1-butene                                                                                           |              | 27.4         | 29.2         | 178.2 | 231.8 | 272.0 | 302.1  |
| 3,3-Dimethyl-1-butene<br>$\Delta H_f = 4.3^{-148.3}$                                                            | 1.1          | 25.7         | 27.1         | 162.8 | 223.4 | 266.1 | 297.1  |
| 2,3-Dimethyl-2-butene<br>$\Delta H_f = 3.5^{-76.3}$                                                             | 5.46         | 29.6         | 32.5         | 156.8 | 216.7 | 262.7 | 297.7  |
| Di(3-methylbutyl) ether                                                                                         |              | 35.2         |              |       |       |       |        |
| Dimethylcadmium                                                                                                 |              |              | 38.0         |       |       |       |        |
| 1,1-Dimethylcyclohexane<br>$\Delta H_f = 6.0^{-120.0}$                                                          | 2.06         | 32.5         | 37.9         | 212.1 | 310.0 | 379.5 | 427.6  |
| <i>cis</i> -1,2-Dimethylcyclohexane<br>$\Delta H_f = 8.3^{-100.6}$                                              | 1.64         | 33.5         | 39.7         | 213.8 | 309.6 | 377.0 | 424.3  |
| <i>trans</i> -1,2-Dimethylcyclohexane                                                                           | 10.49        | 33.0         | 38.4         | 217.2 | 312.1 | 378.7 | 425.5  |
| <i>cis</i> -1,3-Dimethylcyclohexane                                                                             | 10.82        | 32.9         | 38.3         | 214.2 | 310.5 | 378.7 | 426.8  |
| <i>trans</i> -1,3-Dimethylcyclohexane                                                                           | 9.86         | 33.4         | 39.2         | 213.8 | 308.8 | 375.7 | 423.0  |
| <i>cis</i> -1,4-Dimethylcyclohexane                                                                             | 9.31         | 33.3         | 39.0         | 213.8 | 308.8 | 375.7 | 423.0  |
| <i>trans</i> -1,4-Dimethylcyclohexane                                                                           | 12.33        | 32.6         | 37.9         | 215.9 | 312.1 | 378.9 | 425.7  |
| 1,1-Dimethylcyclopentane<br>$\Delta H_f = 6.5^{-126.4}$                                                         | 1.1          | 30.3         | 33.8         | 182.2 | 262.6 | 318.7 | 359.1  |
| <i>cis</i> -1,2-Dimethylcyclopentane<br>$\Delta H_f = 6.7^{-131.7}$                                             | 1.7          | 31.7         | 35.7         | 182.7 | 262.4 | 317.9 | 358.0  |
| <i>trans</i> -1,2-Dimethylcyclopentane                                                                          | 7.2          | 30.9         | 34.6         | 182.9 | 262.2 | 317.3 | 357.4  |
| <i>cis</i> -1,3-Dimethylcyclopentane                                                                            | 7.4          | 30.4         | 34.2         | 182.9 | 262.2 | 317.3 | 357.4  |
| <i>trans</i> -1,3-Dimethylcyclopentane                                                                          | 7.3          | 30.8         | 34.5         | 182.9 | 262.2 | 317.3 | 357.4  |
| <i>cis</i> -2,4-Dimethyl-1,3-dioxane                                                                            |              |              | 39.9         |       |       |       |        |
| 4,5-Dimethyl-1,3-dioxane                                                                                        |              |              | 42.5         |       |       |       |        |
| 5,5-Dimethyl-1,3-dioxane                                                                                        |              |              | 41.3         |       |       |       |        |
| Dimethyl disulfide                                                                                              | 9.19         | 33.8         | 37.9         | 110.3 | 137.4 | 157.6 | 172.8  |
| Dimethyl ether                                                                                                  | 4.94         | 21.5         | 18.5         | 79.6  | 105.3 | 125.7 | 141.4  |
| <i>N,N</i> -Dimethylformamide                                                                                   | 16.15        | 38.4         | 46.9         |       |       |       |        |
| Dimethylglyoxime                                                                                                |              |              | 97.1         |       |       |       |        |
| 2,2-Dimethylheptane                                                                                             | 8.90         |              |              |       |       |       |        |
| 2,6-Dimethyl-4-heptanone                                                                                        |              | 39.9         | 50.9         |       |       |       |        |
| 2,2-Dimethylhexane                                                                                              | 6.78         | 32.1         | 37.3         |       |       |       |        |
| 2,3-Dimethylhexane                                                                                              |              | 33.2         | 38.8         |       |       |       |        |
| 2,4-Dimethylhexane                                                                                              |              | 32.5         | 37.8         |       |       |       |        |
| 2,5-Dimethylhexane                                                                                              | 12.95        | 32.5         | 37.9         |       |       |       |        |
| 3,3-Dimethylhexane                                                                                              | 6.98         | 32.3         | 37.5         |       |       |       |        |
| 3,4-Dimethylhexane                                                                                              |              | 33.2         | 39.0         |       |       |       |        |
| <i>cis</i> -2,2-Dimethyl-3-hexene                                                                               |              |              | 37.2         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                          | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                    |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| <i>trans</i> -2,2-Dimethyl-3-hexene                |              |              | 37.3         |       |       |       |        |
| 1,1-Dimethylhydrazine                              | 10.1         | 32.6         | 35.0         |       |       |       |        |
| 1,2-Dimethylhydrazine                              |              | 35.2         | 39.3         |       |       |       |        |
| 3,5-Dimethylisoxazole                              |              |              | 45.2         |       |       |       |        |
| Dimethyl maleate                                   | 14.7         |              | 44.3         |       |       |       |        |
| Dimethylmercury                                    |              |              | 34.6         |       |       |       |        |
| 6,6-Dimethyl-2-methylene-bicyclo[3.1.1]heptane     |              | 40.2         | 46.4         |       |       |       |        |
| 2,4-Dimethyloctane                                 |              | 36.5         | 47.1         |       |       |       |        |
| Dimethyl oxalate                                   | 21.07        |              | 47.4         |       |       |       |        |
| 3,3-Dimethylloxetane                               |              | 30.9         | 33.9         |       |       |       |        |
| 2,2-Dimethylpentane                                | 5.86         | 29.2         | 32.4         | 211.0 | 285.9 | 340.7 | 381.6  |
| 2,3-Dimethylpentane                                |              | 30.5         | 34.3         | 211.0 | 285.9 | 340.7 | 381.6  |
| 2,4-Dimethylpentane                                | 6.69         | 29.6         | 32.9         | 211.0 | 285.9 | 340.7 | 381.6  |
| 3,3-Dimethylpentane                                | 7.07         | 29.6         | 33.0         | 211.0 | 285.9 | 340.7 | 381.6  |
| 2,2-Dimethyl-3-pentanone                           |              | 36.1         | 42.3         |       |       |       |        |
| 2,4-Dimethyl-3-pentanone                           | 11.18        | 34.6         | 41.5         |       |       |       |        |
| 2,4-Dimethyl-1-pentene                             |              |              | 33.2         |       |       |       |        |
| 4,4-Dimethyl-1-pentene                             |              |              | 29.0         |       |       |       |        |
| 2,4-Dimethyl-2-pentene                             |              |              | 34.4         |       |       |       |        |
| <i>cis</i> -4,4-Dimethyl-2-pentene                 |              |              | 32.7         |       |       |       |        |
| <i>trans</i> -4,4-Dimethyl-2-pentene               |              |              | 32.7         |       |       |       |        |
| 2,7-Dimethylphenanthrene                           |              |              | 106.7        |       |       |       |        |
| 4,5-Dimethylphenanthrene                           |              |              | 104.6        |       |       |       |        |
| 9,10-Dimethylphenanthrene                          |              |              | 119.5        |       |       |       |        |
| 2,3-Dimethylphenol                                 | 21.02        |              | 84.0         |       |       |       |        |
| 2,4-Dimethylphenol                                 |              | 47.1         | 65.0         |       |       |       |        |
| 2,5-Dimethylphenol                                 | 23.38        | 46.9         | 85.0         |       |       |       |        |
| 2,6-Dimethylphenol                                 | 18.90        | 44.5         | 75.3         |       |       |       |        |
| 3,4-Dimethylphenol                                 | 18.13        | 49.7         | 85.0         |       |       |       |        |
| 3,5-Dimethylphenol                                 | 18.00        | 49.3         | 82.0         |       |       |       |        |
| Dimethyl 1,2-phthalate                             | 162.7        |              |              |       |       |       |        |
| 2,2-Dimethylpropane<br>$\Delta H_t = 2.6^{-133.1}$ | 3.10         | 22.7         | 21.8         | 157.1 | 218.5 | 254.3 | 283.7  |
| 2,2-Dimethylpropanenitrile                         |              | 32.4         | 37.3         |       |       |       |        |
| 2,2-Dimethyl-1-propanol                            |              | 9.6          |              |       |       |       |        |
| 2,3-Dimethylpyridine                               |              | 39.1         | 47.7         |       |       |       |        |
| 2,4-Dimethylpyridine                               |              | 38.5         | 47.5         |       |       |       |        |
| 2,5-Dimethylpyridine                               |              |              | 47.8         |       |       |       |        |
| 2,6-Dimethylpyridine                               | 10.04        | 37.5         | 45.4         |       |       |       |        |
| 3,4-Dimethylpyridine                               |              | 40.0         | 50.5         |       |       |       |        |
| 3,5-Dimethylpyridine                               |              | 39.5         | 49.5         |       |       |       |        |
| Dimethyl sulfate                                   |              |              | 48.5         |       |       |       |        |
| Dimethyl sulfide                                   | 7.99         | 27.0         | 27.7         | 88.4  | 113.0 | 132.2 | 147.2  |
| Dimethyl sulfite                                   |              |              | 40.2         |       |       |       |        |
| Dimethyl sulfone                                   |              |              | 77.0         |       |       |       |        |
| Dimethyl sulfoxide                                 | 14.37        | 43.1         | 52.9         |       |       |       |        |
| 2,2-Dimethylthiacyclopropane                       |              |              | 35.8         |       |       |       |        |
| Dimethylzinc                                       |              |              | 29.5         |       |       |       |        |
| Dinitromethane                                     |              |              | 46.0         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                  | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                            |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 2,4-Dinitrophenol          |              |              | 104.6        |       |       |       |        |
| 2,6-Dinitrophenol          |              |              | 112.1        |       |       |       |        |
| 1,1-Dinitropropane         |              |              | 62.5         |       |       |       |        |
| 1,3-Dioxane                |              | 34.4         | 39.1         |       |       |       |        |
| 1,4-Dioxane                | 12.85        | 34.2         | 38.6         | 126.5 | 181.8 | 218.2 | 243.3  |
| $\Delta H_t = 2.4^{-0.3}$  |              |              |              |       |       |       |        |
| 1,3-Dioxolane              | 27.48        |              | 35.6         |       |       |       |        |
| Diphenylamine              | 17.86        |              | 89.1         |       |       |       |        |
| Diphenyl carbonate         | 23.4         |              | 90.0         |       |       |       |        |
| Diphenyl disulfide         |              |              | 95.0         |       |       |       |        |
| Diphenyl disulfone         |              |              | 161.9        |       |       |       |        |
| Diphenylenimine            |              |              | 84.5         |       |       |       |        |
| 1,2-Diphenylethane         |              | 51.5         | 91.4         |       |       |       |        |
| 1,1-Diphenylethylene       |              |              | 73.2         |       |       |       |        |
| Diphenyl ether             | 17.22        | 48.2         | 67.0         |       |       |       |        |
| 6,6-Diphenylfulvene        |              |              | 104.6        |       |       |       |        |
| Diphenylmercury            |              |              | 112.8        |       |       |       |        |
| Diphenylmethane            | 18.2         |              | 67.5         |       |       |       |        |
| 1,3-Diphenyl-2-propanone   |              |              | 89.1         |       |       |       |        |
| Diphenyl sulfide           |              |              | 67.8         |       |       |       |        |
| Diphenyl sulfone           |              |              | 106.3        |       |       |       |        |
| Diphenyl sulfoxide         |              |              | 97.1         |       |       |       |        |
| 1,2-Dipropoxyethane        |              |              | 50.6         |       |       |       |        |
| Dipropylamine              |              | 33.5         | 40.0         |       |       |       |        |
| Dipropyl disulfide         | 13.8         | 41.9         | 54.1         | 186.2 | 298.3 | 350.2 | 390.0  |
| Dipropyl ether             | 8.83         | 31.3         | 35.7         | 196.2 | 262.0 | 311.3 | 348.0  |
| Dipropylmercury            |              |              | 55.2         |       |       |       |        |
| Dipropyl sulfate           |              |              | 66.9         |       |       |       |        |
| Dipropyl sulfide           | 12.1         | 36.6         | 44.2         | 201.7 | 272.5 | 328.2 | 372.6  |
| Dipropyl sulfite           |              |              | 58.6         |       |       |       |        |
| Dipropyl sulfone           |              |              | 79.9         |       |       |       |        |
| Dipropyl sulfoxide         |              |              | 74.5         |       |       |       |        |
| Divinyl ether              |              |              | 26.2         |       |       |       |        |
| Divinyl sulfone            |              |              | 56.5         |       |       |       |        |
| Dodecane                   | 36.55        | 44.5         | 61.5         | 356.2 | 481.3 | 572.2 | 656.5  |
| Dodecanedioic acid         |              |              | 153.1        |       |       |       |        |
| Dodecanenitrile            |              |              | 76.1         |       |       |       |        |
| Dodecanoic acid            | 36.64        |              | 132.6        |       |       |       |        |
| Dodecanol                  | 31.4         | 63.5         | 92.0         |       |       |       |        |
| 1-Dodecene                 | 17.42        | 44.0         | 60.8         | 341.8 | 460.0 | 545.6 | 608.8  |
| $\Delta H_t = 4.6^{-60.2}$ |              |              |              |       |       |       |        |
| 1,2-Epoxybutane            |              | 30.3         |              |       |       |       |        |
| 1,2-Epoxypropane           |              | 21.6         |              |       |       |       |        |
| Ergosterol                 |              |              | 118.4        |       |       |       |        |
| Ethane                     | 2.86         | 14.7         | 5.2          | 65.5  | 89.3  | 108.0 | 122.6  |
| Ethane- $d_6$              |              |              |              | 81.7  | 108.5 | 127.4 | 140.5  |
| 1,2-Ethanediamine          | 22.58        | 38.0         | 45.0         |       |       |       |        |
| 1,2-Ethenediol             | 11.23        | 50.5         | 67.8         | 113.2 | 136.9 | 166.9 |        |
| 1,2-Ethenediol diacetate   |              | 45.5         | 61.4         |       |       |       |        |
| 1,2-Ethanedithiol          |              | 37.9         | 44.7         |       |       |       |        |



**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                              |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Ethanethiol                                  | 4.98         | 26.8         | 27.3         | 88.2  | 113.9 | 133.2 | 148.0  |
| Ethanol                                      | 5.02         | 38.6         | 42.3         | 81.2  | 107.7 | 127.2 | 141.9  |
| Ethanolamine                                 | 20.50        | 49.8         |              |       |       |       |        |
| Ethoxybenzene                                |              | 40.7         | 51.0         |       |       |       |        |
| 2-Ethoxyethanol                              |              | 39.2         | 48.2         |       |       |       |        |
| 2-(2-Ethoxyethoxy)ethanol                    |              | 47.5         |              |       |       |       |        |
| 2-(2-Ethoxyethoxy)ethyl acetate              |              | 91.2         |              |       |       |       |        |
| 2-Ethoxyethyl acetate                        |              |              | 52.7         |       |       |       |        |
| 1-Ethoxy-2-methoxyethane                     |              | 34.3         | 39.8         |       |       |       |        |
| <i>N</i> -Ethylacetamide                     |              |              | 64.9         |       |       |       |        |
| Ethyl acetate                                | 10.48        | 31.9         | 35.6         | 137.4 | 182.6 | 213.4 | 234.5  |
| Ethyl acrylate                               |              | 34.7         |              |       |       |       |        |
| Ethylamine                                   |              | 28.0         | 26.6         | 90.6  | 119.6 | 141.8 | 158.5  |
| <i>N</i> -Ethylaniline                       |              |              | 52.3         |       |       |       |        |
| Ethylbenzene                                 | 9.18         | 35.6         | 42.2         | 170.5 | 236.1 | 281.0 | 312.8  |
| 2-Ethylbenzoic acid                          |              |              | 100.7        |       |       |       |        |
| 3-Ethylbenzoic acid                          |              |              | 99.1         |       |       |       |        |
| 4-Ethylbenzoic acid                          |              |              | 97.5         |       |       |       |        |
| 2-Ethyl-1-butanol                            |              | 43.2         | 63.2         |       |       |       |        |
| Ethyl butanoate                              |              | 35.5         | 42.7         |       |       |       |        |
| 2-Ethylbutanoic acid                         |              | 51.2         |              |       |       |       |        |
| 2-Ethyl-1-butene                             |              | 28.8         | 31.1         | 170.3 | 228.0 | 269.5 | 300.8  |
| Ethyl <i>trans</i> -2-butenolate             |              |              | 44.4         |       |       |       |        |
| Ethyl chloroacetate                          |              | 40.4         | 49.5         |       |       |       |        |
| Ethyl 4-chlorobutanoate                      |              |              | 52.7         |       |       |       |        |
| Ethyl chloroformate                          |              |              | 42.3         |       |       |       |        |
| Ethyl <i>trans</i> -cinnamate                |              | 58.6         |              |       |       |       |        |
| Ethyl crotonate                              |              |              | 44.3         |       |       |       |        |
| Ethyl cyanoacetate                           |              | 64.4         |              |       |       |       |        |
| Ethylcyclobutane                             |              | 28.7         | 31.2         |       |       |       |        |
| Ethylcyclohexane                             | 8.33         | 34.0         | 40.6         | 215.9 | 310.0 | 377.0 | 423.8  |
| 1-Ethylcyclohexene                           |              |              | 43.3         |       |       |       |        |
| Ethylcyclopentane                            | 6.9          | 32.0         | 36.4         | 183.6 | 258.2 | 314.7 | 356.3  |
| 1-Ethylcyclopentene                          |              | 38.5         |              |       |       |       |        |
| Ethyl dichloroacetate                        |              |              | 50.6         |       |       |       |        |
| Ethyl 2,2-dimethylpropanoate                 |              | 34.5         | 41.2         |       |       |       |        |
| Ethylene                                     | 3.35         | 13.5         |              | 53.1  | 70.7  | 83.8  | 93.9   |
| Ethylene- <i>d</i> <sub>4</sub>              |              |              |              | 63.9  | 82.3  | 95.6  | 104.9  |
| Ethylene carbonate                           | 13.19        | 50.1         | 73.2         |       |       |       |        |
| 2,2'-(Ethylenedioxy)bis(ethanol)             |              | 71.4         | 79.1         |       |       |       |        |
| Ethylene glycol ( <i>see</i> 1,2-Ethanediol) |              |              |              |       |       |       |        |
| Ethylene glycol diacetate                    |              |              | 61.4         |       |       |       |        |
| Ethylene oxide                               | 5.2          | 25.5         | 24.8         | 62.6  | 86.3  | 102.9 | 114.9  |
| Ethylenimine                                 |              | 30.3         | 34.6         | 70.4  | 98.6  | 117.7 | 131.6  |
| <i>N</i> -Ethylformamide                     |              |              | 58.4         |       |       |       |        |
| Ethyl formate                                | 9.20         | 29.9         | 32.0         |       |       |       |        |
| 2-Ethylhexanal                               |              |              | 49.0         |       |       |       |        |
| 2-Ethylhexane                                |              | 33.6         | 39.6         |       |       |       |        |
| Ethyl hexanoate                              |              |              | 51.7         |       |       |       |        |
| 2-Ethylhexanoic acid                         |              | 56.0         | 75.6         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                              |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 2-Ethyl-1-hexanol            |              | 45.2         |              |       |       |       |        |
| 2-Ethylhexyl acetate         |              | 43.5         | 48.1         |       |       |       |        |
| 2-Ethyl hydroperoxide        |              |              | 43.1         |       |       |       |        |
| Ethylidenecyclohexane        |              |              | 42.0         |       |       |       |        |
| Ethylidenecyclopentane       |              | 18.1         |              |       |       |       |        |
| Ethyl isocyanide             |              |              | 33.5         |       |       |       |        |
| Ethyl isopentanoate          | 8.7          | 43.9         |              |       |       |       |        |
| Ethyl isopentyl ether        |              | 33.0         | 39.0         |       |       |       |        |
| Ethylisopropylamine          |              | 29.9         | 33.1         |       |       |       |        |
| Ethyl isopropyl ether        |              | 28.2         | 30.1         |       |       |       |        |
| Ethyl isopropyl sulfide      | 8.7          | 32.7         | 37.8         |       |       |       |        |
| Ethyl lactate                |              | 46.4         | 49.4         |       |       |       |        |
| Ethyllithium                 |              |              | 116.7        |       |       |       |        |
| Ethylmercury bromide         |              |              | 76.6         |       |       |       |        |
| Ethylmercury chloride        |              |              | 76.1         |       |       |       |        |
| Ethylmercury iodide          |              |              | 79.5         |       |       |       |        |
| 1-Ethyl-2-methylbenzene      | 10.0         | 38.9         | 47.7         | 202.9 | 275.3 | 326.8 | 363.6  |
| 1-Ethyl-3-methylbenzene      | 7.6          | 38.5         | 46.9         | 198.7 | 273.6 | 325.5 | 363.2  |
| 1-Ethyl-4-methylbenzene      | 13.4         | 38.4         | 46.6         | 197.5 | 272.0 | 324.7 | 362.2  |
| Ethyl 2-methylbutanoate      |              |              | 44.4         |       |       |       |        |
| Ethyl 3-methylbutanoate      |              | 37.0         | 43.9         |       |       |       |        |
| 2-Ethyl-3-methyl-1-butene    |              |              | 34.5         |       |       |       |        |
| 1-Ethyl-1-methylcyclopentane |              | 33.2         | 38.9         |       |       |       |        |
| Ethyl methyl ether           |              | 26.7         |              | 109.1 | 144.7 | 172.3 | 193.2  |
| 3-Ethyl-2-methylpentane      | 11.34        | 32.9         | 38.5         |       |       |       |        |
| 3-Ethyl-3-methylpentane      | 10.84        | 32.8         | 38.0         |       |       |       |        |
| 3-Ethyl-2-methyl-1-pentene   |              |              | 37.5         |       |       |       |        |
| Ethyl 2-methylpropanoate     |              | 33.7         | 39.8         |       |       |       |        |
| Ethyl methyl sulfide         | 9.8          | 29.5         | 31.9         | 116.4 | 152.3 | 179.6 | 200.6  |
| Ethyl nitrate                | 8.5          | 33.1         | 36.3         | 120.2 | 155.1 | 178.7 | 195.4  |
| 1-Ethyl-2-nitrobenzene       |              |              | 59.8         |       |       |       |        |
| 1-Ethyl-4-nitrobenzene       |              |              | 62.8         |       |       |       |        |
| 3-Ethylpentane               | 9.55         | 31.1         | 35.2         | 211.0 | 285.9 | 340.7 | 381.6  |
| Ethyl pentanoate             |              | 37.0         | 47.0         |       |       |       |        |
| Ethyl pentyl ether           |              | 34.4         | 41.0         |       |       |       |        |
| 2-Ethylphenol                |              |              | 63.6         |       |       |       |        |
| 3-Ethylphenol                |              |              | 68.2         |       |       |       |        |
| 4-Ethylphenol                |              |              | 80.3         |       |       |       |        |
| Ethylphosphonic acid         |              |              | 50.6         |       |       |       |        |
| Ethylphosphonic dichloride   |              |              | 42.7         |       |       |       |        |
| Ethyl propanoate             |              | 33.9         | 39.2         |       |       |       |        |
| Ethyl propyl ether           |              | 28.9         | 31.4         |       |       |       |        |
| Ethyl propyl sulfide         | 10.6         | 34.2         | 40.0         | 173.3 | 232.7 | 279.0 | 315.6  |
| Ethyl trichloroacetate       |              |              | 51.0         |       |       |       |        |
| S-Ethyl thiolacetate         | 34.4         | 40.0         |              |       |       |       |        |
| Ethyl 2-vinylacrylate        |              |              | 48.5         |       |       |       |        |
| Ethyl vinyl ether            |              | 26.2         | 26.6         |       |       |       |        |
| Fluoranthrene                | 18.87        |              | 99.2         |       |       |       |        |
| 9H-Fluorene                  | 19.58        |              |              |       |       |       |        |
| Fluorobenzene                | 11.31        | 31.2         | 34.6         | 125.5 | 171.0 | 200.1 | 220.0  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                   | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$   |       |        |        |
|---------------------------------------------|--------------|--------------|--------------|---------|-------|--------|--------|
|                                             |              |              |              | 400 K   | 600 K | 800 K  | 1000 K |
| 4-Fluorobenzoic acid                        |              |              | 91.2         |         |       |        |        |
| Fluoroethane                                |              |              |              | 74.1    | 98.6  | 116.4  | 129.7  |
| Fluoromethane                               |              | 16.7         |              | 44.2    | 57.9  | 68.8   | 77.2   |
| 1-Fluorooctane                              |              | 40.4         | 49.7         |         |       |        |        |
| 1-Fluoropropane                             |              |              |              | 102.7   | 137.3 | 162.7  | 181.5  |
| 2-Fluoropropane                             |              |              |              | 103.5   | 138.7 | 163.8  | 182.2  |
| 2-Fluorotoluene                             |              | 35.4         |              |         |       |        |        |
| 4-Fluorotoluene                             | 9.4          | 34.1         | 39.4         | 152.4   | 207.9 | 245.2  | 271.3  |
| Fluorotrichloromethane                      |              | 25.0         |              |         |       |        |        |
| Fluorotrinitromethane                       |              |              | 34.7         |         |       |        |        |
| Formaldehyde                                |              | 23.3         |              | 39.2(g) | 48.2  | 55.9   | 62.0   |
| Formamide                                   | 6.69         |              | 60.2         |         |       |        |        |
| Formic acid                                 | 12.7         | 22.7         | 20.1         | 53.8    | 67.0  | 76.8   | 83.5   |
| Formyl fluoride                             |              | 21.7         |              | 46.4    | 56.2  | 63.1   | 67.9   |
| Fumaric acid                                |              |              | 136.0        |         |       |        |        |
| Fumaronitrile                               |              |              | 72.0         |         |       |        |        |
| Furan, $\Delta H_t = 2.1^{-123.2}$          | 3.80         | 27.1         | 27.5         | 88.7    | 122.6 | 164.9  | 158.5  |
| 2-Furancarboxaldehyde                       | 14.35        | 43.2         | 50.6         |         |       |        |        |
| 2-Furancarboxylic acid                      |              |              | 108.5        |         |       |        |        |
| Furanmethanol                               | 13.13        | 53.6         | 64.4         |         |       |        |        |
| Glutaric acid                               | 20.9         |              |              |         |       |        |        |
| Glycerol                                    | 18.28        | 61.0         | 85.8         |         |       |        |        |
| Glyceryl triacetate                         |              |              | 85.7         |         |       |        |        |
| Glyceryl tributanoate                       |              |              | 107.1        |         |       |        |        |
| Glyceryl trinitrate                         | 21.87        |              | 100.0        |         |       |        |        |
| Heptadecane, $\Delta H_t = 11.0^{11.1}$     | 40.5         | 52.9         | 86.0         | 501.4   | 676.8 | 803.7  | 897.9  |
| Heptadecanoic acid                          | 58.8         |              |              |         |       |        |        |
| 1-Heptadecene                               | 31.4         | 51.8         | 85.0         | 486.9   | 655.5 | 777.1  | 866.9  |
| 1-Heptanal                                  | 23.6         |              | 47.7         | 213.4   | 283.3 | 333.9  | 371.1  |
| Heptane                                     | 14.16        | 31.8         | 36.6         | 211.0   | 285.9 | 340.7  | 381.6  |
| 1-Heptanenitrile                            |              |              | 51.9         |         |       |        |        |
| 1-Heptanethiol                              | 25.4         | 39.8         | 50.6         | 233.5   | 312.1 | 372.0  | 418.4  |
| Heptanoic acid                              |              |              | 74.0         |         |       |        |        |
| 1-Heptanol                                  | 13.2         | 48.1         | 66.8         | 224.4   | 300.9 | 357.0  | 392.5  |
| 2-Heptanol                                  |              | 49.8         |              |         |       |        |        |
| 3-Heptanol                                  |              | 42.5         |              |         |       |        |        |
| 2-Heptanone                                 |              | 38.3         | 47.2         |         |       |        |        |
| 4-Heptanone                                 |              | 36.2         |              |         |       |        |        |
| 1-Heptene, $\Delta H_t = 0.3^{-136}$        | 12.66        | 31.1         | 35.5         | 196.5   | 264.6 | 314.1  | 351.0  |
| <i>trans</i> -2-Heptene                     | 11.72        |              |              |         |       |        |        |
| Heptylamine                                 |              |              | 50.0         |         |       |        |        |
| Heptyl methyl ether                         |              |              | 46.9         |         |       |        |        |
| Hexachlorobenzene                           | 23.85        |              | 92.6         | 201.2   | 233.4 | 250.9  | 260.8  |
| Hexachloroethane, $\Delta H_t = 8.0^{71.3}$ | 9.8          | 45.9         | 59.0         | 151.5   | 166.6 | 173.6  | 177.3  |
| Hexadecafluoroethylcyclohexane              |              |              | 38.5         |         |       |        |        |
| Hexadecafluoroheptane                       |              |              | 36.4         |         |       |        |        |
| Hexadecane                                  | 51.8         | 51.2         | 81.4         | 472.3   | 687.7 | 757.4  | 846.0  |
| Hexadecanoic acid                           | 42.04        |              | 154.4        |         |       |        |        |
| 1-Hexadecanol, $\Delta H_t = 16.6^{34}$     | 34.29        |              | 169.5        | 485.7   | 652.7 | 773.6  | 863.2  |
| 1-Hexadecene                                | 30.2         | 50.4         | 80.3         | 457.9   | 616.4 | 731.82 | 815.0  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                                                      | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|--------------------------------------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                                                |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Hexadienoic acid                                                               | 13.6         |              |              |       |       |       |        |
| Hexafluoroacetone                                                              |              | 19.8         | 21.3         |       |       |       |        |
| Hexafluoroacetylacetone                                                        |              | 27.1         | 30.6         |       |       |       |        |
| Hexafluorobenzene                                                              | 11.58        | 31.7         | 35.7         | 183.6 | 219.9 | 241.1 | 253.7  |
| Hexafluoroethane, $\Delta H_t = 3.7^{-169.2}$                                  | 2.7          | 16.2         |              | 125.6 | 149.0 | 160.7 | 166.8  |
| <i>cis</i> -Hexahydroindane                                                    |              |              | 57.5         |       |       |       |        |
| <i>trans</i> -Hexahydroindane                                                  |              |              | 56.1         |       |       |       |        |
| Hexamethylbenzene<br>$\Delta H_t = 1.1^{-156.7}$<br>$\Delta H_t = 1.8^{110.7}$ | 20.6         | 48.2         | 74.7         | 310.4 | 406.4 | 474.9 | 525.3  |
| 1,1,1,3,3,3-Hexamethyldisilazane                                               |              |              | 41.4         |       |       |       |        |
| Hexamethyldisiloxane                                                           |              |              | 37.2         |       |       |       |        |
| Hexamethylphosphoric triamide                                                  | 14.28        |              |              |       |       |       |        |
| Hexanal                                                                        |              |              |              | 184.2 | 243.9 | 287.4 | 319.7  |
| Hexanamide                                                                     | 25.1         |              | 98.7         |       |       |       |        |
| Hexane                                                                         | 13.08        | 28.9         | 31.6         | 181.9 | 246.8 | 294.4 | 330.1  |
| 1,6-Hexanedioic acid                                                           | 34.85        |              | 129.3        |       |       |       |        |
| 1,6-Hexanediol                                                                 | 25.5         |              | 83.3         |       |       |       |        |
| Hexanenitrile                                                                  |              | 38.0         | 47.9         |       |       |       |        |
| 1-Hexanethiol                                                                  | 18.0(1)      | 37.2         | 45.8         | 204.5 | 273.1 | 325.1 | 366.7  |
| Hexanoic acid                                                                  | 15.40        | 71.1         | 72.2         |       |       |       |        |
| 1-Hexanol                                                                      | 15.40        | 44.5         | 61.6         | 195.3 | 261.8 | 310.7 | 346.9  |
| 2-Hexanol                                                                      |              | 41.0         | 58.5         |       |       |       |        |
| 3-Hexanol                                                                      | 44.3         | 46.0         |              |       |       |       |        |
| 2-Hexanone                                                                     | 14.90        | 36.4         | 43.1         |       |       |       |        |
| 3-Hexanone                                                                     | 13.49        | 35.4         | 42.5         |       |       |       |        |
| 1-Hexene                                                                       | 9.35         | 28.3         | 30.6         | 167.5 | 225.5 | 267.9 | 299.3  |
| <i>cis</i> -2-Hexene                                                           | 8.86         | 29.1         | 32.2         | 161.5 | 221.8 | 165.3 | 297.9  |
| <i>trans</i> -2-Hexene                                                         | 8.26         | 28.9         | 31.6         | 166.1 | 223.4 | 266.1 | 297.9  |
| <i>cis</i> -3-Hexene                                                           | 8.25         | 28.7         | 31.4         | 161.1 | 222.6 | 265.7 | 297.9  |
| <i>trans</i> -3-Hexene                                                         | 11.08        | 28.9         | 31.7         | 168.2 | 225.5 | 267.4 | 298.7  |
| Hexylamine                                                                     |              | 36.5         | 45.1         |       |       |       |        |
| Hexyl methyl ether                                                             |              | 34.9         | 42.1         |       |       |       |        |
| 1-Hexyne                                                                       |              |              |              | 158.5 | 207.5 | 243.3 | 270.1  |
| Hydrazine                                                                      | 12.7         | 45.3         |              |       |       |       |        |
| 2-Hydroxybenzaldehyde                                                          |              | 38.2         |              |       |       |       |        |
| 2-Hydroxybenzoic acid                                                          |              |              | 95.1         |       |       |       |        |
| 2-Hydroxy-2,4,6-cycloheptatrienone                                             |              |              | 83.7         |       |       |       |        |
| 2-Hydroxy-1-isopropyl-4-methylbenzene                                          |              |              | 91.2         |       |       |       |        |
| 4-Hydroxy-4-methyl-2-pentanone                                                 |              | 28.5         | 47.7         |       |       |       |        |
| 3-Hydroxypropanonitrile                                                        |              | 56.1         |              |       |       |       |        |
| 2-Hydroxypyridine                                                              |              |              | 86.6         |       |       |       |        |
| 3-Hydroxypyridine                                                              |              |              | 88.3         |       |       |       |        |
| 4-Hydroxypyridine                                                              |              |              | 103.8        |       |       |       |        |
| 8-Hydroxyquinoline                                                             |              |              | 108.8        |       |       |       |        |
| Icosane                                                                        | 69.88        | 57.5         | 100.8        | 588.5 | 794.0 | 942.6 | 1052.7 |
| Icosanoic acid                                                                 | 72.0         |              | 199.6        |       |       |       |        |
| 1-Icosene                                                                      | 34.3         | 55.9         | 99.8         | 574.0 | 772.7 | 916.0 | 1021.7 |
| Indane                                                                         |              | 39.6         | 48.8         |       |       |       |        |
| Indene                                                                         |              |              | 52.9         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                   | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|-----------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                             |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Indole                      |              |              | 69.9         |       |       |       |        |
| Iodobenzene                 | 9.76         | 39.5         | 47.7         | 130.1 | 173.3 | 201.1 | 220.1  |
| Iodobenzoic acid            |              |              | 87.9         |       |       |       |        |
| 1-Iodobutane                |              | 34.7         | 40.6         |       |       |       |        |
| 2-Iodobutane                |              | 33.3         | 38.5         |       |       |       |        |
| Iodocyclohexane             |              |              | 47.3         |       |       |       |        |
| Iodoethane                  |              | 29.4         | 31.9         | 80.3  | 103.1 | 119.9 | 132.4  |
| 1-Iodohexane                |              |              | 49.8         |       |       |       |        |
| Iodomethane                 |              | 27.3         | 28.0         | 51.6  | 63.9  | 73.1  | 80.2   |
| 1-Iodo-2-methylpropane      |              | 33.5         | 38.8         |       |       |       |        |
| 2-Iodo-2-methylpropane      | 14.5         | 31.4         | 35.4         | 148.8 | 191.7 | 221.1 | 242.3  |
| 1-Iodonaphthalene           |              |              | 72.4         |       |       |       |        |
| 2-Iodonaphthalene           |              |              | 90.8         |       |       |       |        |
| 1-Iodopentane               |              |              | 45.3         |       |       |       |        |
| 1-Iodopropane               |              | 32.1         | 36.2         | 109.9 | 142.7 | 166.5 | 184.2  |
| 2-Iodopropane               |              | 30.7         | 34.1         | 111.2 | 144.7 | 168.2 | 185.5  |
| 3-Iodo-1-propene            |              |              | 38.1         |       |       |       |        |
| 2-Iodotoluene (also 3-, 4-) |              |              | 54.4         |       |       |       |        |
| Isobutanonitrile            |              | 32.4         | 37.2         | 119.5 | 156.4 | 183.0 | 202.5  |
| Isobutyl acetate            |              | 35.9         |              |       |       |       |        |
| Isobutylamine               |              | 30.6         | 33.9         |       |       |       |        |
| Isobutylbenzene             | 12.51        | 37.8         | 47.9         |       |       |       |        |
| Isobutylcyclohexane         |              |              | 47.6         |       |       |       |        |
| Isobutyl dichloroacetate    |              |              | 52.3         |       |       |       |        |
| Isobutyl formate            |              | 33.6         |              |       |       |       |        |
| Isobutyl isobutanoate       |              | 38.2         | 46.4         |       |       |       |        |
| Isobutyl isopropyl ether    |              | 31.6         | 36.6         |       |       |       |        |
| Isobutyl methyl ether       |              | 28.0         | 30.1         |       |       |       |        |
| Isobutyl propyl ether       |              | 28.3         | 30.3         |       |       |       |        |
| Isobutyl trichloroacetate   |              |              | 53.1         |       |       |       |        |
| Isobutyl vinyl ether        |              | 30.7         | 34.6         |       |       |       |        |
| 2-Isopropoxyethanol         |              | 40.4         | 50.1         |       |       |       |        |
| Isopropyl acetate           |              | 32.9         | 37.2         |       |       |       |        |
| Isopropylamine              | 7.33         | 27.8         | 28.4         |       |       |       |        |
| Isopropylbenzene            | 7.79         | 37.5         | 45.1         | 200.8 | 277.0 | 328.9 | 365.3  |
| Isopropylcyclohexane        |              |              | 44.0         |       |       |       |        |
| Isopropylcyclopentane       |              | 33.6         | 39.4         |       |       |       |        |
| Isopropylmethylamine        |              | 28.7         | 30.9         |       |       |       |        |
| 1-Isopropyl-2-methylbenzene | 10.0         | 38.4         | 50.6         |       |       |       |        |
| 1-Isopropyl-3-methylbenzene | 13.7         | 38.1         | 50.0         |       |       |       |        |
| 1-Isopropyl-4-methylbenzene | 9.7          | 38.2         | 50.2         |       |       |       |        |
| Isopropyl methyl ether      |              | 26.1         | 26.4         | 138.0 | 184.8 | 220.4 | 247.2  |
| 2-Isopropyl-5-methylphenol  |              |              | 91.2         |       |       |       |        |
| Isopropyl methyl sulfide    | 9.4          | 30.7         | 34.2         | 145.1 | 192.5 | 229.9 | 260.6  |
| Isopropyl nitrate           |              | 34.9         | 38.8         | 150.5 | 195.9 | 226.5 | 247.9  |
| Isopropylpropylamine        |              | 32.1         | 37.2         |       |       |       |        |
| Isopropyl propyl sulfide    |              | 35.1         | 41.8         |       |       |       |        |
| Isopropyl trichloroacetate  |              |              | 51.9         |       |       |       |        |
| Isoquinoline                | 7.45         | 49.0         | 60.3         |       |       |       |        |
| Ketene                      |              |              | 20.4         | 59.5  | 70.7  | 78.7  | 86.4   |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                             | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|-------------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                       |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| (-)-Leucine                                           |              |              | 150.6        |       |       |       |        |
| (+)-Limonene                                          |              |              | 48.1         |       |       |       |        |
| Maleic acid                                           |              |              | 110.0        |       |       |       |        |
| Maleic anhydride                                      |              |              | 71.5         |       |       |       |        |
| Malononitrile                                         |              |              | 79.1         |       |       |       |        |
| D-Mannitol                                            | 22.6         |              |              |       |       |       |        |
| Methacrylonitrile                                     |              | 31.8         |              |       |       |       |        |
| Methane                                               | 0.94         | 8.2          |              | 40.5  | 52.2  | 62.9  | 71.8   |
| Methane- $d_4$                                        |              |              |              | 48.6  | 63.4  | 74.8  | 83.0   |
| Methanethiol, $\Delta H_t = 0.22^{-135.6}$            | 5.91         | 24.6         | 23.8         | 58.7  | 73.5  | 85.0  | 94.1   |
| Methanol, $\Delta H_t = 0.6^{-115.8}$                 | 3.18         | 35.2         | 37.4         | 51.4  | 67.0  | 79.7  | 89.5   |
| 4-Methoxybenzaldehyde                                 |              | 56.8         | 64.5         |       |       |       |        |
| Methoxybenzene                                        |              | 39.0         | 46.9         |       |       |       |        |
| 2-Methoxybenzoic acid                                 |              |              | 104.7        |       |       |       |        |
| 3-Methoxybenzoic acid                                 |              |              | 107.4        |       |       |       |        |
| 4-Methoxybenzoic acid                                 |              |              | 109.8        |       |       |       |        |
| 3-Methoxy-1-butanol                                   |              | 50.8         |              |       |       |       |        |
| 2-Methoxyethanol                                      |              | 37.5         | 45.2         |       |       |       |        |
| 2-(2-Methoxyethoxy)ethanol                            |              | 46.6         |              |       |       |       |        |
| 2-Methoxyethyl acetate                                |              | 43.9         | 50.3         |       |       |       |        |
| 2-Methoxy-1-propoxyethane                             |              | 36.3         | 43.7         |       |       |       |        |
| 2-Methoxytetrahydropyran                              |              |              | 42.7         |       |       |       |        |
| 1-Methoxy-2,4,6-trinitrobenzene                       |              |              | 133.1        |       |       |       |        |
| N-Methylacetamide                                     | 9.72         | 59.4         |              |       |       |       |        |
| Methyl acetate                                        |              | 30.3         | 32.3         |       |       |       |        |
| Methyl acetoacetate                                   |              | 36.0         |              |       |       |       |        |
| Methyl acrylate                                       |              | 33.1         | 29.2         |       |       |       |        |
| Methylamine                                           | 6.13         | 25.6         | 24.4         | 60.2  | 78.9  | 93.9  | 105.7  |
| 4-Methylaniline                                       | 18.22        |              |              |       |       |       |        |
| Methyl benzoate                                       | 9.74         | 43.2         | 55.6         |       |       |       |        |
| 2-Methylbenzoic acid                                  | 20.17        |              |              |       |       |       |        |
| 3-Methylbenzoic acid                                  | 15.72        |              |              |       |       |       |        |
| 4-Methylbenzoic acid                                  | 22.73        |              |              |       |       |       |        |
| 1-Methylbicyclo[4.1.0]heptane                         |              |              | 39.2         |       |       |       |        |
| 1-Methylbicyclo[3.1.0]hexane                          |              | 31.1         | 34.8         |       |       |       |        |
| 2-Methyl-1,3-butadiene                                | 4.79         | 25.9         | 26.8         | 133.1 | 173.2 | 200.8 | 221.3  |
| 3-Methyl-1,3-butadiene                                |              | 27.2         | 28.0         | 129.7 | 168.6 | 197.5 | 219.2  |
| 2-Methylbutane                                        | 5.15         | 24.7         | 24.9         | 152.7 | 208.7 | 249.8 | 280.8  |
| 3-Methylbutanenitrile                                 |              | 35.1         | 41.7         |       |       |       |        |
| 2-Methylbutanethiol                                   |              | 33.8         | 39.5         |       |       |       |        |
| 3-Methyl-1-butanethiol                                | 7.5          |              | 39.4         |       |       |       |        |
| 2-Methyl-2-butanethiol<br>$\Delta H_t = 8.0^{-114.0}$ | 0.6          | 31.4         | 35.7         | 179.0 | 236.7 | 279.4 | 308.8  |
| Methyl butanoate                                      |              | 33.8         | 39.3         |       |       |       |        |
| 2-Methylbutanoic acid                                 |              |              | 46.9         |       |       |       |        |
| 3-Methylbutanoic acid                                 | 7.32         | 43.2         | 57.5         |       |       |       |        |
| 2-Methyl-1-butanol                                    |              | 45.2         | 55.2         |       |       |       |        |
| 3-Methyl-1-butanol                                    |              | 44.1         | 55.6         |       |       |       |        |
| 2-Methyl-2-butanol, $\Delta H_t = 2.0^{-127.2}$       | 4.45         | 39.0         | 50.1         |       |       |       |        |
| 3-Methyl-2-butanol                                    |              | 41.8         | 53.0         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                      | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|--------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 3-Methyl-2-butanone            |              | 32.4         | 36.8         |       |       |       |        |
| 2-Methyl-1-butene              | 7.9          | 25.5         | 25.9         | 138.9 | 187.1 | 222.4 | 248.7  |
| 3-Methyl-1-butene              | 5.4          | 24.1         | 23.8         | 147.5 | 192.1 | 225.3 | 250.3  |
| 2-Methyl-2-butene              | 7.6          | 26.3         | 27.1         | 133.6 | 181.7 | 217.8 | 245.0  |
| Methyl 2-butenolate            |              |              | 41.0         |       |       |       |        |
| 3-Methyl-1-butyne              |              | 26.2         | 25.8         | 130.1 | 169.9 | 198.3 | 219.2  |
| 2-Methylbutyl acetate          |              | 37.5         |              |       |       |       |        |
| Methyl chloroacetate           |              | 39.2         | 46.7         |       |       |       |        |
| Methyl cyanoacetate            |              | 48.2         | 61.7         |       |       |       |        |
| Methyl cyclobutanecarboxylate  |              | 37.1         | 44.7         |       |       |       |        |
| Methylcyclohexane              | 6.75         | 31.3         | 35.4         | 185.6 | 269.7 | 329.5 | 371.5  |
| 1-Methylcyclohexanol           |              | 79.0         | 80           |       |       |       |        |
| cis-2-Methylcyclohexanol       |              | 48.5         | 63.2         |       |       |       |        |
| trans-2-Methylcyclohexanol     |              | 53.0         | 63.2         |       |       |       |        |
| cis-3-Methylcyclohexanol       |              |              | 65.3         |       |       |       |        |
| trans-3-Methylcyclohexanol     |              |              | 65.3         |       |       |       |        |
| cis-4-Methylcyclohexanol       |              |              | 65.7         |       |       |       |        |
| trans-4-Methylcyclohexanol     |              |              | 66.1         |       |       |       |        |
| 1-Methylcyclohexene            |              |              | 37.9         |       |       |       |        |
| Methylcyclopentane             | 6.93         | 29.1         | 31.6         | 151.1 | 219.4 | 267.8 | 303.1  |
| 1-Methyl-1-cyclopentene        |              |              | 32.6         | 136.0 | 195.8 | 238.5 | 269.0  |
| 3-Methyl-1-cyclopentene        |              |              | 31.0         | 136.4 | 197.1 | 239.3 | 269.9  |
| 4-Methyl-1-cyclopentene        |              |              | 32.2         | 136.4 | 196.7 | 238.4 | 269.5  |
| Methyl cyclopropanecarboxylate |              | 35.3         | 41.3         |       |       |       |        |
| 2-Methyldecane                 |              | 40.3         | 54.3         |       |       |       |        |
| 4-Methyldecane                 |              | 40.7         | 53.8         |       |       |       |        |
| Methyl decanoate               |              |              | 66.7         |       |       |       |        |
| Methyl dichloroacetate         |              | 39.3         | 47.7         |       |       |       |        |
| Methyldichlorosilane           |              |              | 28.0         |       |       |       |        |
| Methyl 2,2-dimethylpropanoate  |              | 33.4         | 38.8         |       |       |       |        |
| 2-Methyl-1,3-dioxane           |              |              | 38.6         |       |       |       |        |
| 4-Methyl-1,3-dioxane           |              |              | 39.2         |       |       |       |        |
| 4-Methyl-1,3-dioxolan-2-one    | 9.62         |              |              |       |       |       |        |
| Methyl dodecanoate             |              |              | 77.2         |       |       |       |        |
| N-Methylethanediamine          |              | 37.6         | 45.2         |       |       |       |        |
| 1-Methylethyl acetate          |              | 32.9         | 37.3         |       |       |       |        |
| 1-Methylethyl thiolacetate     |              | 35.7         | 42.3         |       |       |       |        |
| N-Methylformamide              |              |              | 56.2         |       |       |       |        |
| Methyl formate                 | 7.45         | 27.9         | 28.4         | 81.6  | 105.4 | 121.8 | 133.9  |
| Methyl 2-furancarboxylate      |              |              | 45.2         |       |       |       |        |
| Methylglyoxal                  |              |              | 38.1         |       |       |       |        |
| 2-Methylheptane                | 11.88        | 33.3         | 39.7         |       |       |       |        |
| 3-Methylheptane                | 11.38        | 33.7         | 39.8         |       |       |       |        |
| 4-Methylheptane                | 10.84        | 33.4         | 39.7         |       |       |       |        |
| Methyl heptanoate              |              |              | 51.6         |       |       |       |        |
| 2-Methylhexane                 | 8.87         | 30.6         | 34.9         | 211.0 | 285.9 | 340.7 | 381.6  |
| 3-Methylhexane                 |              | 30.9         | 35.1         | 212.0 | 285.9 | 340.7 | 381.6  |
| Methyl hexanoate               |              | 38.6         | 48.0         |       |       |       |        |
| 5-Methyl-1-hexene              |              |              | 34.3         |       |       |       |        |
| cis-3-Methyl-3-hexene          |              |              | 36.5         |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                         | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|---------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                   |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| <i>trans</i> -3-Methyl-3-hexene                   |              |              | 35.9         |       |       |       |        |
| Methylhydrazine                                   | 10.4         | 36.1         | 40.4         |       |       |       |        |
| Methyl isobutanoate                               |              | 32.6         | 37.3         |       |       |       |        |
| Methyl isocyanide                                 |              |              | 30.8         |       |       |       |        |
| 1-Methyl-4-isopropylbenzene                       | 9.60         | 38.2         |              |       |       |       |        |
| 3-Methylisoxazole                                 |              |              | 41.0         |       |       |       |        |
| 5-Methylisoxazole                                 |              |              | 41.0         |       |       |       |        |
| Methylmercury bromide                             |              |              | 67.8         |       |       |       |        |
| Methylmercury chloride                            |              |              | 64.4         |       |       |       |        |
| Methylmercury iodide                              |              |              | 65.3         |       |       |       |        |
| Methyl methacrylate                               |              | 36.0         | 60.7         |       |       |       |        |
| Methyl 2-methylbutanoate                          |              |              | 41.8         |       |       |       |        |
| Methyl-3-methylbutanoate                          |              |              | 41.0         |       |       |       |        |
| 1-Methylnaphthalene<br>$\Delta H_t = 5.0^{-32.4}$ | 6.94         | 45.5         |              | 212.3 | 292.0 | 345.1 | 381.6  |
| 2-Methylnaphthalene<br>$\Delta H_t = 5.6^{15.4}$  | 11.97        | 46.0         | 61.7         | 211.2 | 290.0 | 343.2 | 381.2  |
| Methyl nitrate                                    | 8.2          | 31.6         | 32.1         | 91.5  | 115.2 | 131.7 | 143.1  |
| Methyl nitrite                                    |              | 20.9         | 22.6         | 76.3  | 97.7  | 112.8 | 123.5  |
| 1-Methyl-4-nitrobenzene                           |              |              | 79.1         |       |       |       |        |
| 2-Methylnonane                                    |              | 38.2         | 49.6         |       |       |       |        |
| 3-Methylnonane                                    |              | 38.3         | 49.7         |       |       |       |        |
| 5-Methylnonane                                    |              | 38.1         | 49.3         |       |       |       |        |
| 2-Methyloctane                                    | 18.00        |              |              |       |       |       |        |
| Methyl octanoate                                  |              |              | 56.4         |       |       |       |        |
| Methyl oxirane                                    |              | 27.4         | 27.9         |       |       |       |        |
| 2-Methylpentane                                   | 6.27         | 27.8         | 29.9         | 184.1 | 211.7 | 296.2 | 331.4  |
| 3-Methylpentane                                   | 5.30         | 28.1         | 30.3         | 181.9 | 246.9 | 294.6 | 330.1  |
| 2-Methyl-2,4-pentanediol                          |              | 57.3         |              |       |       |       |        |
| 3-Methylpentanenitrile                            |              | 35.1         | 41.6         |       |       |       |        |
| Methyl pentanoate                                 |              | 35.4         | 43.1         |       |       |       |        |
| 2-Methylpentanoic acid                            |              | 52.1         | 57.5         |       |       |       |        |
| 2-Methyl-1-pentanol                               |              | 50.2         | 55.7         |       |       |       |        |
| 2-Methyl-2-pentanol                               |              | 39.6         | 54.8         |       |       |       |        |
| 2-Methyl-3-pentanol                               |              | 41.8         | 54.4         |       |       |       |        |
| 3-Methyl-1-pentanol                               |              | 46.3         | 62.3         |       |       |       |        |
| 3-Methyl-2-pentanol                               |              | 43.4         | 56.9         |       |       |       |        |
| 4-Methyl-1-pentanol                               |              | 44.5         | 60.5         |       |       |       |        |
| 4-Methyl-2-pentanol                               |              | 44.2         | 50.6         |       |       |       |        |
| 3-Methyl-3-pentanol                               |              | 41.8         |              |       |       |       |        |
| 2-Methyl-3-pentanone                              |              | 33.8         | 39.8         |       |       |       |        |
| 3-Methyl-2-pentanone                              |              | 34.2         | 40.5         |       |       |       |        |
| 4-Methyl-2-pentanone                              |              | 34.5         | 40.6         |       |       |       |        |
| 2-Methyl-1-pentene                                |              | 28.1         | 30.5         | 170.7 | 227.6 | 269.5 | 300.4  |
| 3-Methyl-1-pentene                                |              | 26.9         | 28.7         | 177.8 | 232.6 | 272.8 | 302.5  |
| 4-Methyl-1-pentene                                |              | 27.1         | 28.7         | 162.8 | 221.3 | 264.0 | 296.2  |
| 2-Methyl-2-pentene                                |              | 29.0         | 31.6         | 163.2 | 222.6 | 245.2 | 297.5  |
| <i>cis</i> -3-Methyl-2-pentene                    |              | 28.8         | 31.2         | 163.2 | 222.6 | 265.3 | 297.5  |
| <i>trans</i> -3-Methyl-2-pentene                  |              | 29.3         | 31.5         | 163.2 | 222.6 | 265.3 | 297.5  |
| <i>cis</i> -4-Methyl-2-pentene                    |              | 27.6         | 29.5         | 167.6 | 226.4 | 267.8 | 299.2  |



**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                             | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |       |       |        |
|---------------------------------------|--------------|--------------|--------------|----------|-------|-------|--------|
|                                       |              |              |              | 400 K    | 600 K | 800 K | 1000 K |
| <i>trans</i> -4-Methyl-2-pentene      |              | 28.0         | 30.0         | 171.1    | 229.3 | 269.9 | 300.4  |
| 4-Methyl-3-penten-2-one               |              | 36.1         |              | 214.0    |       |       |        |
| Methyl pentyl ether                   |              | 32.0         | 36.9         |          |       |       |        |
| Methyl pentyl sulfide                 |              | 37.4         | 45.2         | 203.6    | 272.2 | 324.6 | 366.0  |
| 3-Methyl-1-phenyl-1-butanone          |              |              | 59.5         |          |       |       |        |
| 2-Methyl-1-phenylpropane              | 12.5         | 37.8         | 49.5         |          |       |       |        |
| Methyl phenyl sulfide                 |              |              | 54.3         |          |       |       |        |
| Methyl phenyl sulfone                 |              |              | 92.0         |          |       |       |        |
| Methylphosphonic acid                 |              |              | 48.1         |          |       |       |        |
| 2-Methylpiperidine                    |              |              | 40.5         |          |       |       |        |
| 2-Methylpropanal                      |              |              | 31.5         |          |       |       |        |
| 2-Methylpropane                       | 4.66         | 21.3         | 19.3         | 124.6    | 169.5 | 202.9 | 227.6  |
| 2-Methylpropanenitrile                |              | 32.4         | 37.1         |          |       |       |        |
| 2-Methyl-1-propanethiol               | 5.0          | 31.0         | 34.6         | 147.7    | 193.6 | 225.0 | 247.6  |
| 2-Methyl-2-propanethiol               | 2.5          | 28.5         | 30.8         | 151.2    | 199.2 | 232.3 | 256.2  |
| $\Delta H_t = 4.1^{-121.6}$           |              |              |              |          |       |       |        |
| $\Delta H_t = 0.7^{-116.2}$           |              |              |              |          |       |       |        |
| $\Delta H_t = 1.0^{-73.8}$            |              |              |              |          |       |       |        |
| Methyl propanoate                     |              | 32.2         | 35.9         |          |       |       |        |
| 2-Methylpropanoic acid                | 5.02         |              | 35.3         |          |       |       |        |
| 2-Methyl-1-propanol                   | 6.32         | 41.8         | 50.8         |          |       |       |        |
| 2-Methyl-2-propanol                   | 6.79         | 39.1         | 46.7         | 142.9    | 189.8 | 222.9 | 247.5  |
| $\Delta H_t = 0.8^{13}$               |              |              |              |          |       |       |        |
| 2-Methylpropene                       | 5.93         | 22.1         | 20.6         | 111.2    | 147.7 | 175.1 | 196.0  |
| Methyl propyl ether                   |              | 26.8         | 27.6         | 138.1    | 183.8 | 218.7 | 244.8  |
| Methyl propyl sulfide                 | 9.9          | 32.1         | 36.2         | 144.9    | 191.9 | 227.8 | 255.8  |
| 2-Methylpyridine                      | 9.72         | 36.2         | 42.5         | 133.6    | 186.4 | 222.6 | 243.3  |
| 3-Methylpyridine                      | 14.18        | 37.4         | 44.4         | 133.1    | 186.1 | 222.3 | 247.8  |
| 4-Methylpyridine                      | 11.57        | 37.5         | 44.6         |          |       |       |        |
| 1-Methyl-1 <i>H</i> -pyrrole          |              |              | 40.8         |          |       |       |        |
| Methyl salicylate                     |              | 46.7         |              |          |       |       |        |
| $\alpha$ -Methylstyrene               |              |              |              | 187.4    | 254.0 | 300.4 | 333.9  |
| <i>cis</i> - $\beta$ -Methylstyrene   |              |              |              | 187.4    | 254.0 | 300.4 | 333.9  |
| <i>trans</i> - $\beta$ -Methylstyrene |              |              |              | 189.1    | 256.1 | 301.3 | 334.7  |
| Methyl tetradecanoate                 |              |              | 37.0         |          |       |       |        |
| 2-Methylthiacyclopentane              |              | 36.4         | 41.8         |          |       |       |        |
| 4-Methylthiazole                      |              | 37.6         | 43.8         |          |       |       |        |
| 2-Methylthiophene                     | 9.20         | 33.9         | 38.9         | 123.1    | 165.6 | 194.3 | 214.6  |
| 3-Methylthiophene                     | 10.53        | 34.2         | 39.4         | 122.9    | 164.6 | 192.3 | 211.7  |
| Methyl trichloroacetate               |              |              | 48.3         |          |       |       |        |
| Methyl tridecanoate                   |              |              | 82.7         |          |       |       |        |
| Methyl undecanoate                    |              |              | 71.4         |          |       |       |        |
| 5-Methyluracil                        |              |              | 134.1        |          |       |       |        |
| Morpholine                            |              | 37.1         | 44.0         |          |       |       |        |
| Naphthalene                           | 18.98        | 43.2         | 72.6         | 180.1(g) | 251.5 | 297.3 | 329.2  |
| 1-Naphthalenecarboxylic acid          |              |              | 110.4        |          |       |       |        |
| 2-Naphthalenecarboxylic acid          |              |              | 113.6        |          |       |       |        |
| 1-Naphthol                            | 23.33        |              | 91.2         |          |       |       |        |
| 2-Naphthol                            | 17.51        |              | 94.2         |          |       |       |        |
| 1,4-Naphthoquinone                    |              |              | 72.4         |          |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                          |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 1-Naphthylamine                          |              |              | 90.0         |       |       |       |        |
| 2-Naphthylamine                          |              |              | 88.3         |       |       |       |        |
| 2-Nitroaniline                           | 16.11        |              | 90.0         |       |       |       |        |
| 3-Nitroaniline                           | 23.68        |              | 96.7         |       |       |       |        |
| 4-Nitroaniline                           | 21.1         |              | 109          |       |       |       |        |
| Nitrobenzene                             | 11.59        | 40.8         | 55.0         |       |       |       |        |
| 1-Nitrobutane                            |              | 38.9         | 48.6         | 157.5 | 210.1 | 247.0 | 273.6  |
| 2-Nitrobutane                            |              | 36.8         | 43.8         | 157.4 | 211.1 | 248.7 | 276.0  |
| Nitroethane                              | 9.85         | 38.0         | 41.6         | 99.0  | 131.6 | 154.0 | 170.2  |
| Nitromethane                             | 9.70         | 34.0         | 38.3         | 70.3  | 91.7  | 106.9 | 117.9  |
| (Nitromethyl)benzene                     |              |              | 53.6         |       |       |       |        |
| 2-Nitrophenol                            | 17.44        |              |              |       |       |       |        |
| 3-Nitrophenol                            | 19.2         |              |              |       |       |       |        |
| 4-Nitrophenol                            | 18.25        |              |              |       |       |       |        |
| 1-Nitronaphthalene                       |              |              | 107.1        |       |       |       |        |
| 1-Nitropropane                           |              | 38.5         | 43.4         | 128.5 | 171.0 | 200.7 | 222.0  |
| 2-Nitropropane                           |              | 36.8         | 41.3         | 129.2 | 172.3 | 201.8 | 222.8  |
| 2-Nitroso-1-naphthol                     |              |              | 56.5         |       |       |       |        |
| 4-Nitroso-1-naphthol                     |              |              | 87.4         |       |       |       |        |
| 1-Nitroso-2-naphthol                     |              |              | 86.6         |       |       |       |        |
| 2-Nitrotoluene                           |              | 16.5         | 47.2         |       |       |       |        |
| 3-Nitrotoluene                           |              | 15.0         | 49.9         |       |       |       |        |
| 4-Nitrotoluene                           | 16.81        | 15.5         | 50.2         |       |       |       |        |
| Nonadecane, $\Delta H_t = 13.8^{22.8}$   | 45.82        | 56.0         | 95.8         | 559.4 | 754.9 | 896.3 | 1000.8 |
| 1-Nonadecene                             | 33.5         | 54.6         | 94.9         | 545.0 | 733.7 | 869.7 | 969.9  |
| 1-Nonal                                  |              |              | 72.3         | 271.1 | 361.5 | 426.4 | 474.5  |
| Nonane, $\Delta H_t = 6.3^{-56.0}$       | 15.47        | 36.9         | 46.4         | 269.0 | 364.1 | 433.3 | 484.9  |
| 1-Nonanethiol                            | 33.5         | 44.4         |              | 291.6 | 390.3 | 464.6 | 521.5  |
| Nonanoic acid                            | 20.28        |              | 82.4         |       |       |       |        |
| 1-Nonanol                                |              | 54.4         | 76.9         | 282.4 | 379.1 | 449.6 | 501.7  |
| 2-Nonanone                               |              |              | 56.4         |       |       |       |        |
| 5-Nonanone                               | 24.93        |              | 53.3         |       |       |       |        |
| 1-Nonene                                 | 18.08        | 36.3         | 45.5         | 254.6 | 342.8 | 406.8 | 454.0  |
| cis-Octadecafluorodecahydronaphthalene   |              | 35.6         | 45.2         |       |       |       |        |
| trans-Octadecafluorodecahydronaphthalene |              | 35.8         | 45.4         |       |       |       |        |
| Octadecafluoropropylcyclohexane          |              |              | 24.5         |       |       |       |        |
| Octadecafluorooctane                     |              | 33.4         | 41.1         |       |       |       |        |
| Octadecane                               | 61.39        | 54.5         | 152.8        | 530.4 | 715.8 | 850.0 | 949.4  |
| Octadecanedioic acid                     | 56.6         |              |              |       |       |       |        |
| Octadecanoic acid                        | 56.59        |              | 166.5        |       |       |       |        |
| Octadecanol                              |              |              | 113.4        |       |       |       |        |
| 1-Octadecene                             | 32.6         | 53.3         | 90.0         | 516.0 | 694.5 | 823.4 | 918.4  |
| cis-9-Octadecenoic acid                  |              | 64.7         |              |       |       |       |        |
| Octafluorocyclobutane                    | 2.77         | 23.2         |              | 186.1 | 225.3 | 245.4 | 257.3  |
| Octafluorotoluene                        | 11.58        |              |              |       |       |       |        |
| Octamethylcyclotetrasiloxane             |              | 45.6         |              |       |       |       |        |
| Octanal                                  |              |              |              | 242.3 | 322.2 | 380.3 | 422.6  |
| Octanamide                               |              |              | 110.5        |       |       |       |        |
| Octane                                   | 20.65        | 34.4         | 41.5         | 240.0 | 325.0 | 387.0 | 433.5  |
| 1,8-Octanedioic acid                     |              |              | 143.1        |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                                                          | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------------------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                                                    |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Octanenitrile                                                                      |              | 41.3         | 56.8         |       |       |       |        |
| 1-Octanethiol                                                                      | 24.3         | 42.3         |              | 262.6 | 351.3 | 418.3 | 469.9  |
| Octanoic acid                                                                      | 21.36        | 58.5         | 81.7         |       |       |       |        |
| 1-Octanol                                                                          | 42.30        | 46.9         | 71.0         | 253.4 | 340.0 | 403.3 | 450.1  |
| (±)-2-Octanol                                                                      |              | 44.4         |              |       |       |       |        |
| (±)-3-Octanol                                                                      |              | 36.5         |              |       |       |       |        |
| 4-Octanol                                                                          |              | 40.5         |              |       |       |       |        |
| 2-Octanone                                                                         | 24.42        |              |              |       |       |       |        |
| 1-Octene                                                                           | 15.57        | 34.1         | 40.4         | 225.6 | 303.7 | 360.5 | 402.5  |
| 1-Octyne                                                                           |              | 35.8         | 42.3         | 216.5 | 285.7 | 336.0 | 410.9  |
| 2-Octyne                                                                           |              | 37.3         | 44.5         |       |       |       |        |
| 3-Octyne                                                                           |              | 36.9         | 43.9         |       |       |       |        |
| 4-Octyne                                                                           |              | 36.0         | 42.7         |       |       |       |        |
| Oxalic acid                                                                        |              |              | 98.0         |       |       |       |        |
| Oxaloyl chloride                                                                   |              |              | 31.8         |       |       |       |        |
| Oxamide                                                                            |              |              | 113.0        |       |       |       |        |
| Oxetane                                                                            |              | 28.7         | 29.9         |       |       |       |        |
| 2-Oxetanone                                                                        |              |              | 47.0         |       |       |       |        |
| 2-Oxohexamethyleneimine                                                            | 16.2         | 54.8         | 83.3         |       |       |       |        |
| 4-Oxopentanoic acid                                                                | 9.22         |              |              |       |       |       |        |
| 1,1'-Oxybis(2-ethoxy)ethane                                                        |              |              | 58.4         |       |       |       |        |
| 2,2'-Oxybis(ethanol)                                                               |              | 52.3         | 57.3         |       |       |       |        |
| Paraldehyde                                                                        |              |              | 41.4         |       |       |       |        |
| Pentachloroethane                                                                  | 11.34        | 36.9         | 45.6         | 133.7 | 152.1 | 162.0 | 168.1  |
| Pentachlorofluoroethane                                                            | 1.9          |              |              |       |       |       |        |
| Pentachlorophenol                                                                  |              |              | 67.4         |       |       |       |        |
| Pentacyclo-<br>[4.2.0.0 <sup>2,5</sup> .0 <sup>3,8</sup> .0 <sup>4,7</sup> ]octane |              |              | 80.3         |       |       |       |        |
| Pentadecane, $\Delta H_t = 9.2^{-2.25}$                                            | 34.8         | 49.5         | 76.1         | 443.3 | 598.6 | 711.1 | 794.5  |
| Pentadecanoic acid                                                                 | 50.2         |              | 162.7        |       |       |       |        |
| 1-Pentadecene                                                                      | 28.9         | 48.7         | 75.1         | 428.9 | 577.3 | 684.5 | 763.6  |
| 1,2-Pentadiene                                                                     |              | 27.6         | 28.7         | 131.4 | 170.7 | 199.6 | 220.9  |
| cis-1,3-Pentadiene                                                                 |              | 27.6         | 28.3         | 123.4 | 166.9 | 196.7 | 218.4  |
| trans-1,3-Pentadiene                                                               |              | 27.0         | 27.8         | 130.5 | 171.1 | 199.6 | 220.1  |
| 1,4-Pentadiene                                                                     | 6.14         | 25.2         | 25.7         | 131.0 | 170.2 | 220.5 |        |
| 2,3-Pentadiene                                                                     |              | 28.2         | 29.5         | 125.1 | 164.9 | 195.0 | 217.6  |
| Pentaerythritol                                                                    |              | 92           | 143.9        |       |       |       |        |
| Pentaerythritol tetranitrate                                                       |              |              | 151.9        |       |       |       |        |
| Pentafluorobenzene                                                                 | 10.85        | 32.2         | 36.3         |       |       |       |        |
| Pentafluorobenzoic acid                                                            |              |              | 91.6         |       |       |       |        |
| Pentafluoroethane                                                                  |              |              |              | 113.8 | 137.8 | 151.1 | 158.9  |
| Pentafluorophenol                                                                  | 12.85        |              | 67.4         |       |       |       |        |
| 2,3,4,5,6-Pentafluorotoluene                                                       | 12.99        | 34.8         | 41.1         |       |       |       |        |
| Pentamethylbenzene                                                                 | 12.3         | 45.1         | 60.8         | 272.0 | 360.2 | 423.8 | 470.0  |
| $\Delta H_t = 2.0^{23.7}$                                                          |              |              |              |       |       |       |        |
| 2,2,4,6,6-Pentamethylheptane                                                       |              |              | 49.0         |       |       |       |        |
| Pentanal                                                                           |              |              | 38.8         | 155.2 | 205.0 | 241.4 | 267.8  |
| Pentanamide                                                                        |              |              | 89.3         |       |       |       |        |
| Pentane                                                                            | 8.42         | 25.8         | 26.4         | 152.8 | 207.7 | 248.1 | 278.5  |
| 1,5-Pentanediol                                                                    |              | 60.7         |              |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                          | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                    |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 1,5-Pentanedithiol                 |              |              | 59.3         |       |       |       |        |
| 2,4-Pentanedione                   |              | 34.3         | 41.8         |       |       |       |        |
| Pentanenitrile                     | 4.73         | 36.1         | 43.6         |       |       |       |        |
| 1-Pentanethiol                     | 17.5         | 34.9         | 41.2         | 175.4 | 234.0 | 279.4 | 315.1  |
| Pentanoic acid                     | 14.16        | 44.1         | 62.4         |       |       |       |        |
| 1-Pentanol                         | 9.83         | 44.4         | 57.0         | 166.3 | 222.8 | 264.4 | 295.4  |
| 2-Pentanol                         |              | 41.4         | 54.2         |       |       |       |        |
| 3-Pentanol                         |              | 43.5         | 54.0         |       |       |       |        |
| 2-Pentanone                        | 10.63        | 33.4         | 38.4         | 152.4 | 202.2 | 239.0 | 266.1  |
| 3-Pentanone                        | 11.59        | 33.5         | 38.5         |       |       |       |        |
| 1-Pentene                          | 5.81         | 25.2         | 25.5         | 138.5 | 186.4 | 221.5 | 247.7  |
| cis-2-Pentene                      | 7.12         | 26.1         | 26.9         | 132.1 | 182.5 | 218.8 | 245.9  |
| trans-2-Pentene                    | 8.36         | 26.1         | 26.8         | 136.7 | 184.2 | 219.5 | 246.1  |
| cis-2-Pentenitrile                 |              | 36.4         | 43.2         |       |       |       |        |
| trans-2-Pentenitrile               |              | 37.8         | 44.9         |       |       |       |        |
| trans-3-Pentenitrile               |              | 37.1         | 44.8         |       |       |       |        |
| Pentyl acetate                     |              | 41.0         |              |       |       |       |        |
| Pentylamine                        |              | 34.0         | 40.1         |       |       |       |        |
| Pentylcyclohexane                  |              |              | 53.9         |       |       |       |        |
| Pentyl propyl ether                |              | 35.0         | 42.8         |       |       |       |        |
| 1-Pentyne                          |              | 27.7         | 28.4         | 130.1 | 169.0 | 197.1 | 218.4  |
| 2-Pentyne                          |              | 29.3         | 30.8         | 122.2 | 161.9 | 192.1 | 215.1  |
| Perylene                           | 31.75        |              |              |       |       |       |        |
| $\alpha$ -Phellandrene             |              |              | 50.6         |       |       |       |        |
| Phenanthrene                       | 16.46        | 55.7         | 75.5         |       |       |       |        |
| 9,10-Phenanthrenedione             |              |              | 91.6         |       |       |       |        |
| Phenazine                          |              |              | 99.9         |       |       |       |        |
| Phenol                             | 11.29        | 45.7         | 57.8         | 135.8 | 182.2 | 211.8 | 232.2  |
| Phenyl acetate                     |              |              | 54.8         |       |       |       |        |
| Phenylacetonitrile                 |              | 52.9         |              |       |       |       |        |
| Phenylacetylene                    |              |              | 41.8         | 150.4 | 200.9 | 233.4 | 255.9  |
| (-)-3-Phenyl-1-alanine             |              |              | 155.2        |       |       |       |        |
| $\alpha$ -Phenylbenzeneacetic acid | 31.27        |              |              |       |       |       |        |
| Phenyl benzoate                    |              |              | 99.0         |       |       |       |        |
| Phenylboron dichloride             |              |              | 33.9         |       |       |       |        |
| Phenylcyclopropane                 |              |              | 50.2         |       |       |       |        |
| N-Phenyldiacetimide                |              |              | 90.0         |       |       |       |        |
| Phenyl formate                     |              |              | 52.9         |       |       |       |        |
| Phenylhydrazine                    | 16.43        |              | 61.7         |       |       |       |        |
| 1-Phenyl-1-propanone               |              |              | 58.5         |       |       |       |        |
| 1-Phenyl-2-propanone               |              |              | 49.0         |       |       |       |        |
| Phenyl salicylate                  |              |              | 92.1         |       |       |       |        |
| Phenyl vinyl ether                 |              |              | 49.9         |       |       |       |        |
| Phthalamide                        |              |              | 57.3         |       |       |       |        |
| 1,3-Phthalic acid                  |              |              | 106.7        |       |       |       |        |
| 1,4-Phthalic acid                  |              |              | 98.3         |       |       |       |        |
| Phthalic anhydride                 |              |              | 88.7         |       |       |       |        |
| Phthalonitrile                     |              |              | 86.9         |       |       |       |        |
| Piperidine                         | 14.85        | 31.7         | 39.3         |       |       |       |        |
| Propadiene                         |              | 18.6         |              | 72.0  | 92.1  | 106.4 | 117.2  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                   | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|---------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                             |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Propanal                                    |              | 28.3         | 29.6         | 96.6  | 126.4 | 148.3 | 164.0  |
| Propanamide                                 | 17.6         |              | 85.9         |       |       |       |        |
| Propane                                     | 3.53         | 19.0         | 14.8         | 94.0  | 128.7 | 154.8 | 174.6  |
| 1,2-Propanediamine                          |              |              | 44.2         |       |       |       |        |
| 1,3-Propanediamine                          |              | 40.9         | 50.2         |       |       |       |        |
| Propanedinitrile                            |              |              | 79.1         |       |       |       |        |
| 1,2-Propanediol                             |              | 54.1         | 58.0         |       |       |       |        |
| 1,3-Propanediol                             |              | 57.9         | 37.1         |       |       |       |        |
| 1,2-Propanedione                            |              |              | 38.1         |       |       |       |        |
| 1,2-Propanedithiol                          |              |              | 49.7         |       |       |       |        |
| Propanenitrile, $\Delta H_t = 1.7^{-96.2}$  | 5.05         | 31.8         | 36.0         | 88.6  | 114.7 | 134.5 | 149.4  |
| 1-Propanethiol, $\Delta H_t = 4.0^{-131.1}$ | 5.5          | 29.5         | 31.9         | 116.6 | 153.6 | 182.4 | 205.1  |
| 2-Propanethiol                              | 5.7          | 27.9         | 29.5         | 118.6 | 154.9 | 181.0 | 200.5  |
| 1,2,3-Propanetriol triacetate               |              | 57.8         | 85.7         |       |       |       |        |
| 1,2,3-Propanetriol trinitrate               | 21.9         |              |              |       |       |       |        |
| Propanoic acid                              | 10.66        | 32.3         | 32.1         |       |       |       |        |
| Propanoic anhydride                         |              | 41.7         | 52.6         |       |       |       |        |
| 1-Propanol                                  | 5.20         | 41.4         | 47.4         | 108.2 | 144.6 | 171.7 | 192.2  |
| 2-Propanol                                  | 5.37         | 39.9         | 45.4         | 112.0 | 149.6 | 176.3 | 195.9  |
| Propanolactone                              |              |              | 47.0         |       |       |       |        |
| 2-Propenal                                  |              | 28.3         | 31.3         |       |       |       |        |
| Propene                                     | 3.00         | 18.4         | 14.2         | 80.5  | 108.0 | 128.7 | 144.4  |
| 2-Propenenitrile                            | 6.23         |              |              |       |       |       |        |
| Propenoic acid                              | 11.16        |              |              |       |       |       |        |
| 2-Propen-1-ol                               |              | 40.0         | 47.3         | 95.4  | 126.0 | 147.6 | 163.4  |
| cis-1-Propenylbenzene                       |              |              |              | 187.4 | 254.0 | 300.4 | 333.9  |
| 2-Propoxyethanol                            |              | 41.4         | 52.1         |       |       |       |        |
| Propyl acetate                              |              | 33.9         | 39.7         |       |       |       |        |
| 1-Propylamine                               | 10.97        | 29.6         | 31.3         | 119.3 | 159.0 | 188.0 | 210.1  |
| Propylbenzene                               | 9.27         | 38.2         | 46.2         | 200.1 | 275.6 | 327.6 | 364.7  |
| Propyl benzoate                             |              | 49.8         | 51.9         |       |       |       |        |
| Propyl carbamate                            |              |              | 81.2         |       |       |       |        |
| Propyl chloroacetate                        |              |              | 48.5         |       |       |       |        |
| Propylcyclohexane                           | 10.37        | 36.1         | 45.1         | 247.3 | 350.6 | 423.4 | 474.5  |
| Propylcyclopentane                          | 10.0         | 34.7         | 41.1         | 212.7 | 297.2 | 361.0 | 407.9  |
| Propylene oxide                             | 6.5          | 27.4         | 28.3         | 92.7  | 125.8 | 149.3 | 166.5  |
| Propyl formate                              |              | 33.6         | 37.5         |       |       |       |        |
| Propyl nitrate                              |              | 35.9         | 40.6         | 149.8 | 194.5 | 225.4 | 247.2  |
| Propyl propanoate                           |              | 35.5         | 43.5         |       |       |       |        |
| Propyl trichloroacetate                     |              |              | 53.1         |       |       |       |        |
| Propyl vinyl ether                          |              |              | 29.3         |       |       |       |        |
| Propyne                                     |              | 22.1         |              | 72.5  | 91.2  | 105.2 | 115.9  |
| 2-Propyn-1-ol                               |              | 42.1         |              |       |       |       |        |
| Pyrazine                                    |              |              | 56.3         |       |       |       |        |
| Pyrene                                      | 17.11        |              |              |       |       |       |        |
| Pyridazine                                  |              |              | 53.5         |       |       |       |        |
| Pyridine                                    | 8.28         | 35.1         | 40.2         | 106.4 | 149.5 | 177.8 | 197.4  |
| Pyrimidine                                  |              | 49.8         | 50.0         |       |       |       |        |
| 1 <i>H</i> -Pyrrole                         | 7.91         | 38.8         | 45.1         |       |       |       |        |
| Pyrrolidine, $\Delta H_t = 0.5^{-66}$       | 8.58         | 33.0         | 37.6         | 114.4 | 168.7 | 206.5 | 233.6  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                              | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                        |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Quinoline                              | 10.66        | 49.7         | 53.9         |       |       |       |        |
| Salicylic acid                         |              |              | 95.1         |       |       |       |        |
| 5,5'-Spirobis(1,3-dioxane)             |              |              | 72.8         |       |       |       |        |
| Spiro[2.2]pentane                      | 5.8          | 26.8         | 27.5         | 119.5 | 167.8 | 200.5 | 223.9  |
| <i>cis</i> -Stilbene                   |              |              | 69.0         |       |       |       |        |
| <i>trans</i> -Stilbene                 | 27.4         |              | 99.2         |       |       |       |        |
| Styrene                                | 11.0         | 38.7         | 43.9         | 160.3 | 218.2 | 256.9 | 284.2  |
| Succinic acid                          | 32.95        |              | 117.5        |       |       |       |        |
| Succinic anhydride                     | 20.41        |              |              |       |       |       |        |
| Succinonitrile                         | 3.92         |              |              |       |       |       |        |
| <i>p</i> -Terphenyl                    | 35.5         |              |              |       |       |       |        |
| 1,1,2,2-Tetrabromoethane               |              | 48.7         | 70.0         |       |       |       |        |
| Tetrabromomethane                      |              | 45.1         | 110          | 97.1  | 102.6 | 106.7 | 105.9  |
| Tetrabutyltin                          |              |              | 19.8         |       |       |       |        |
| Tetracene                              |              |              | 125.5        |       |       |       |        |
| Tetrachloro-1,4-benzoquinone           |              |              | 98.7         |       |       |       |        |
| 1,1,2,2-Tetrachloro-1,2-difluoroethane | 3.70         | 35.0         |              |       |       |       |        |
| 1,1,1,2-Tetrachloro-2,2-fluorooctane   | 3.99         |              |              |       |       |       |        |
| 1,1,1,2-Tetrachloroethane              |              |              |              | 118.7 | 139.2 | 151.6 | 159.7  |
| 1,1,2,2-Tetrachloroethane              |              | 37.6         | 45.7         | 116.7 | 137.7 | 150.0 | 158.0  |
| Tetrachloroethylene                    | 10.56        | 34.7         | 39.7         | 105.0 | 116.6 | 122.6 | 125.8  |
| Tetrachloromethane                     | 3.28         | 29.8         | 32.4         | 91.7  | 99.7  | 103.1 | 104.8  |
| $\Delta H_t = 4.6^{-47.9}$             |              |              |              |       |       |       |        |
| Tetracyanoethylene                     |              |              | 81.2         |       |       |       |        |
| Tetracyanomethane                      |              |              | 61.1         |       |       |       |        |
| Tetradecane                            | 45.6         | 47.6         | 71.3         | 414.3 | 559.5 | 664.8 | 743.1  |
| Tetradecanenitrile                     |              |              | 85.3         |       |       |       |        |
| Tetradecanoic acid                     | 45.38        |              | 139.8        |       |       |       |        |
| 1-Tetradecanol                         | 49.0         |              | 102.2        |       |       |       |        |
| 1-Tetradecene                          | 27.6         | 46.9         | 70.2         | 399.8 | 538.2 | 638.2 | 712.1  |
| Tetraethylene glycol                   |              | 62.6         | 98.7         |       |       |       |        |
| Tetraethylgermanium                    |              |              | 44.8         |       |       |       |        |
| Tetraethyllead                         |              |              | 56.9         |       |       |       |        |
| Tetraethylsilane                       | 13.01        |              |              |       |       |       |        |
| Tetraethyltin                          |              |              | 51.0         |       |       |       |        |
| 1,1,1,2-Tetrafluoroethane              |              |              |              | 104.2 | 128.7 | 143.1 | 152.1  |
| Tetrafluoroethylene                    | 7.7          | 16.8         |              | 91.9  | 106.8 | 115.5 | 120.8  |
| Tetrafluoromethane                     | 0.7          | 12.6         |              | 72.4  | 86.8  | 94.5  | 98.8   |
| $\Delta H_t = 1.5^{-196.9}$            |              |              |              |       |       |       |        |
| Tetrahydrofuran                        | 8.54         | 29.8         | 32.0         |       |       |       |        |
| Tetrahydrofuran-2,5-dimethanol         |              | 63.6         |              |       |       |       |        |
| Tetrahydrofuran-2-methanol             |              | 45.2         | 51.6         |       |       |       |        |
| 1,2,3,4-Tetrahydronaphthalene          | 12.45        | 43.9         | 55.2         |       |       |       |        |
| Tetrahydropyran                        |              | 31.2         | 34.6         |       |       |       |        |
| Tetrahydropyran-2-methanol             |              | 44.4         |              |       |       |       |        |
| Tetrahydrothiophene                    |              | 34.7         | 39.4         |       |       |       |        |
| Tetrahydrothiophene-1,1-dioxide        | 1.43         |              |              |       |       |       |        |
| Tetraiodomethane                       |              |              |              | 100.4 | 104.4 | 105.9 | 106.7  |
| Tetramethoxysilane                     |              | 194.6        |              |       |       |       |        |
| 1,2,3,4-Tetramethylbenzene             | 11.2         | 45.0         | 57.2         | 237.7 | 316.7 | 374.1 | 416.2  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                              | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                        |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 1,2,3,5-Tetramethylbenzene             | 10.7         | 43.8         | 53.7         | 233.3 | 313.0 | 371.5 | 414.3  |
| 1,2,4,5-Tetramethylbenzene             | 21.0         | 45.5         | 53.4         | 232.2 | 311.2 | 369.9 | 413.0  |
| 2,2,3,3-Tetramethylbutane              | 7.54         | 31.4         | 42.9         |       |       |       |        |
| $\Delta H_t = 2.0^{-120.7}$            |              |              |              |       |       |       |        |
| Tetramethylene sulfone                 | 1.4          | 61.5         |              |       |       |       |        |
| Tetramethyllead                        |              |              | 38.1         |       |       |       |        |
| 2,2,3,3-Tetramethylpentane             | 2.33         |              |              |       |       |       |        |
| 2,2,3,4-Tetramethylpentane             | 0.50         |              |              |       |       |       |        |
| 2,2,4,4-Tetramethylpentane             | 9.75         | 32.5         | 38.5         |       |       |       |        |
| 2,3,3,4-Tetramethylpentane             | 9.00         |              |              |       |       |       |        |
| Tetramethylsilane                      | 6.88         |              |              |       |       |       |        |
| Tetramethyltin                         |              |              | 33.1         |       |       |       |        |
| 1,1,3,3-Tetramethylurea                | 14.10        | 45.6         |              |       |       |       |        |
| Tetranitromethane                      |              | 40.7         | 49.9         |       |       |       |        |
| Tetraphenylmethane                     |              |              | 150.6        |       |       |       |        |
| Tetraphenyltin                         |              |              | 66.3         |       |       |       |        |
| Tetrapropylgermanium                   |              |              | 61.5         |       |       |       |        |
| Tetrapropyltin                         |              |              | 66.9         |       |       |       |        |
| 1,2,3,4-(1 <i>H</i> )-Tetrazole        |              |              | 97.5         |       |       |       |        |
| Thiacyclobutane                        |              | 32.3         | 36.0         |       |       |       |        |
| Thiacycloheptane                       |              |              | 47.3         | 175.7 | 272.0 | 330.5 | 368.2  |
| Thiacyclohexane                        | 2.5          | 36.0         | 42.6         | 149.4 | 219.1 | 267.8 | 302.7  |
| $\Delta H_t = 1.1^{-71.8}$             |              |              |              |       |       |       |        |
| $\Delta H_t = 7.8^{-33.1}$             |              |              |              |       |       |       |        |
| Thiacyclopentane                       | 7.4          | 34.7         | 39.5         | 121.1 | 167.5 | 199.4 | 222.3  |
| Thiacyclopropane                       |              | 29.2         | 30.3         | 69.2  | 92.0  | 107.2 | 118.0  |
| Thioacetamide                          |              |              | 83.3         |       |       |       |        |
| Thioacetic acid                        |              |              | 37.2         | 93.1  | 111.8 | 127.2 | 136.5  |
| 1,2-Thiocresol                         |              |              | 51.5         |       |       |       |        |
| 2,2'-Thiodiethanol                     |              | 66.8         |              |       |       |       |        |
| Thiophene, $\Delta H_t = 0.6^{-101.6}$ | 5.09         | 31.5         | 34.7         | 96.3  | 129.5 | 150.7 | 165.4  |
| Thiophenol                             | 11.5         | 39.9         | 47.6         | 137.1 | 184.6 | 215.9 | 237.6  |
| Thymol                                 | 17.27        |              |              |       |       |       |        |
| Toluene                                | 6.85         | 33.2         | 38.0         | 140.1 | 197.5 | 236.9 | 264.9  |
| <i>o</i> -Toluidine                    |              | 44.6         | 56.7         |       |       |       |        |
| <i>m</i> -Toluidine                    | 3.89         | 44.9         | 57.3         |       |       |       |        |
| <i>p</i> -Toluidine                    | 18.22        | 44.3         |              |       |       |       |        |
| Triacetamide                           |              |              | 60.4         |       |       |       |        |
| 2,4,6-Triamino-1,3,5-triazine          |              |              | 124.3        |       |       |       |        |
| Tribromomethane                        |              | 39.7         | 46.1         | 78.7  | 88.0  | 93.3  | 96.7   |
| Tributoxyborane                        |              | 56.1         | 52.3         |       |       |       |        |
| Tributyl phosphate                     |              | 61.4         | 72.0         |       |       |       |        |
| Trichloroacetic acid                   | 5.88         |              |              |       |       |       |        |
| Trichloroacetonitrile                  |              | 34.1         |              |       |       |       |        |
| Trichloroacetyl chloride               |              |              | 41.0         |       |       |       |        |
| 1,3,5-Trichlorobenzene                 | 18.2         |              |              |       |       |       |        |
| Trichlorobenzquinone                   |              |              | 88.7         |       |       |       |        |
| 1,1,1-Trichloroethane                  | 2.73         | 29.9         | 32.5         | 107.6 | 128.4 | 141.1 | 149.8  |
| $\Delta H_t = 7.5^{-49.0}$             |              |              |              |       |       |       |        |
| 1,1,2-Trichloroethane                  | 11.54        | 34.8         | 40.2         | 104.7 | 126.1 | 139.2 | 148.2  |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                              |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Trichloroethylene                            |              | 31.4         | 34.5         | 91.2  | 104.9 | 112.7 | 117.8  |
| Trichloromethane                             | 8.8          | 29.2         | 31.3         | 74.3  | 85.3  | 91.5  | 95.5   |
| Trichloromethylsilane                        | 8.94         |              |              |       |       |       |        |
| 1,2,3-Trichloropropane                       | 8.9          | 37.1         |              | 31.7  | 38.9  | 43.8  | 47.3   |
| 1,1,1-Trichlorotrifluoroethane               |              | 26.9         | 28.1         |       |       |       |        |
| 1,1,2-Trichlorotrifluoroethane               | 2.47         | 27.0         | 28.4         |       |       |       |        |
| 1,1,1-Trichloro-3,3,3-trifluoropropane       |              | 32.2         | 36.8         |       |       |       |        |
| Tricyanoethylene                             |              |              | 81.2         |       |       |       |        |
| Tridecane, $\Delta H_t = 7.7^{18.2}$         | 28.50        | 45.7         | 66.4         | 385.2 | 520.4 | 618.5 | 691.2  |
| Tridecanenitrile                             |              |              | 85.3         |       |       |       |        |
| Tridecanoic acid                             | 43.1         |              | 146.4        |       |       |       |        |
| 1-Tridecene                                  | 22.83        | 45.0         | 65.3         | 370.8 | 499.1 | 592.0 | 660.2  |
| Triethanolamine                              | 27.2         | 67.5         |              |       |       |       |        |
| Triethoxyborane                              |              |              | 43.9         |       |       |       |        |
| Triethoxymethane                             |              |              | 46.0         |       |       |       |        |
| Triethylaluminum                             |              |              | 73.2         |       |       |       |        |
| Triethylamine                                |              | 31.0         | 34.8         | 203.8 | 276.6 | 328.7 | 367.4  |
| Triethylaminoborane                          |              |              | 60.7         |       |       |       |        |
| Triethylarsine                               |              |              | 43.1         |       |       |       |        |
| Triethyl arsenite                            |              |              | 50.6         |       |       |       |        |
| Triethylbismuthine                           |              |              | 46.0         |       |       |       |        |
| Triethylborane                               |              |              | 36.8         |       |       |       |        |
| Triethylenediamine                           | 6.1          |              | 61.9         |       |       |       |        |
| $\Delta H_t = 9.6^{79.8}$                    |              |              |              |       |       |       |        |
| Triethylene glycol                           |              | 71.4         | 79.1         |       |       |       |        |
| Triethylphosphine                            |              |              | 39.8         |       |       |       |        |
| Triethyl phosphate                           |              |              | 57.3         |       |       |       |        |
| Triethyl phosphite                           |              |              | 41.8         |       |       |       |        |
| Triethylstibine                              |              |              | 43.5         |       |       |       |        |
| Trifluoroacetic acid                         |              | 33.3         | 38.5         |       |       |       |        |
| $\Delta H(\text{dimer dissoc}) = 58.8^{100}$ |              |              |              |       |       |       |        |
| Trifluoroacetonitrile                        | 5.0          |              |              |       |       |       |        |
| 1,1,1-Trifluoro-2-bromo-2-chloroethane       |              | 28.1         | 29.6         |       |       |       |        |
| 1,1,1-Trifluoroethane                        | 6.19         | 19.2         |              | 95.2  | 118.7 | 133.8 | 144.1  |
| 2,2,2-Trifluoroethanol                       |              | 40.0         |              |       |       |       |        |
| Trifluoroethylene                            |              |              |              | 81.1  | 97.5  | 107.5 | 113.9  |
| Trifluoromethane                             | 4.1          | 16.7         |              | 61.1  | 76.0  | 85.1  | 91.0   |
| (Trifluoromethyl)benzene                     | 13.46        | 32.6         | 37.6         | 169.8 | 226.8 | 262.6 | 286.4  |
| Triiodomethane                               | 16.3         |              | 69.9         | 82.0  | 90.0  | 94.7  | 97.8   |
| Triisopropylborane                           |              |              | 41.8         |       |       |       |        |
| Triisopropyl phosphite                       |              |              | 46.0         |       |       |       |        |
| Trimethoxyborane                             |              |              | 34.7         |       |       |       |        |
| 1,1,1-Trimethoxyethane                       |              |              | 39.2         |       |       |       |        |
| Trimethoxymethane                            |              |              | 38.1         |       |       |       |        |
| 2',4',5'-Trimethylacetophenone               |              |              | 63.2         |       |       |       |        |
| 2',4',6'-Trimethylacetophenone               |              |              | 62.3         |       |       |       |        |
| Trimethylaluminum                            |              |              | 63.2         |       |       |       |        |
| Trimethylamine                               | 6.55         | 22.9         | 21.7         | 117.5 | 160.4 | 190.9 | 213.3  |
| Trimethyl arsenite                           |              |              | 42.3         |       |       |       |        |
| Trimethylarsine                              |              |              | 28.9         |       |       |       |        |



**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                                                                          | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|------------------------------------------------------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                                                                    |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| 1,2,3-Trimethylbenzene<br>$\Delta H_t = 0.7^{-54.5}$<br>$\Delta H_t = 1.3^{-42.9}$ | 8.37         | 40.0         | 49.1         | 196.2 | 267.8 | 320.9 | 359.4  |
| 1,2,4-Trimethylbenzene                                                             |              | 39.3         | 47.9         | 196.5 | 269.0 | 321.9 | 360.2  |
| 1,3,5-Trimethylbenzene                                                             | 9.51         | 39.0         | 47.5         | 194.2 | 268.1 | 321.5 | 360.1  |
| 2,6,6-Trimethylbicyclo[3.1.1]-2-heptene                                            |              |              | 44.8         |       |       |       |        |
| Trimethylbismuthine                                                                |              |              | 34.7         |       |       |       |        |
| Trimethylborane                                                                    |              |              | 20.2         |       |       |       |        |
| 2,2,3-Trimethylbutane<br>$\Delta H_t = 2.5^{-151.8}$                               | 2.20         | 28.9         | 32.0         | 212.7 | 291.3 | 346.1 | 386.3  |
| 2,3,3-Trimethyl-1-butene                                                           |              |              | 32.2         |       |       |       |        |
| cis,cis-1,3,5-Trimethylcyclohexane                                                 |              |              |              | 242.9 | 351.2 | 427.6 | 482.0  |
| Trimethylene oxide                                                                 |              | 28.7         | 29.9         |       |       |       |        |
| Trimethylene sulfide<br>$\Delta H_t = 0.7^{-96.5}$                                 | 8.3          | 32.3         | 36.0         | 91.6  | 127.4 | 152.3 | 170.2  |
| Trimethylgallium                                                                   |              |              | 38.1         |       |       |       |        |
| 2,2,5-Trimethylhexane                                                              | 6.2          | 33.7         | 40.2         |       |       |       |        |
| 2,3,5-Trimethylhexane                                                              | 10.00        | 34.4         | 41.4         |       |       |       |        |
| Trimethylindium                                                                    |              |              | 48.5         |       |       |       |        |
| 2,4,7-Trimethyloctane                                                              |              | 38.2         | 49.9         |       |       |       |        |
| 2,2,3-Trimethylpentane                                                             | 8.62         | 31.9         | 36.9         |       |       |       |        |
| 2,2,4-Trimethylpentane                                                             | 9.04         | 30.8         | 35.1         |       |       |       |        |
| 2,3,3-Trimethylpentane<br>$\Delta H_t = 7.7^{-109.0}$                              | 0.86         | 32.1         | 37.3         |       |       |       |        |
| 2,3,4-Trimethylpentane                                                             | 9.27         | 32.4         | 37.7         |       |       |       |        |
| 2,2,4-Trimethyl-1,3-pentanediol                                                    | 8.6          | 55.7         |              |       |       |       |        |
| 2,2,4-Trimethyl-3-pentanone                                                        |              | 35.6         | 43.3         |       |       |       |        |
| 2,4,4-Trimethyl-1-pentene                                                          |              | 31.4         | 35.8         |       |       |       |        |
| 2,4,4-Trimethyl-2-pentene                                                          |              | 32.6         | 37.5         |       |       |       |        |
| Trimethylphosphine                                                                 |              |              | 28.0         |       |       |       |        |
| Trimethylphosphine oxide                                                           |              |              | 50.2         |       |       |       |        |
| Trimethyl phosphate                                                                |              |              | 36.8         |       |       |       |        |
| 2,3,6-Trimethylpyridine                                                            |              | 40.0         | 50.6         |       |       |       |        |
| 2,4,6-Trimethylpyridine                                                            | 9.53         | 39.9         | 50.3         |       |       |       |        |
| Trimethylsilanol                                                                   |              |              | 45.6         |       |       |       |        |
| Trimethylstibine                                                                   |              |              | 31.4         |       |       |       |        |
| Trimethylsuccinic anhydride                                                        |              |              | 74.1         |       |       |       |        |
| Trimethylthiacyclopropane                                                          |              |              | 39.3         |       |       |       |        |
| Trimethyltin bromide                                                               |              |              | 47.3         |       |       |       |        |
| 2,4,6-Trinitroanisole                                                              |              |              | 133.1        |       |       |       |        |
| 1,3,5-Trinitrobenzene                                                              | 16.7         |              | 99.6         |       |       |       |        |
| Trinitromethane                                                                    |              | 32.6         | 46.7         |       |       |       |        |
| 2,4,6-Trinitrophenetole                                                            |              |              | 120.5        |       |       |       |        |
| 2,4,6-Trinitrotoluene                                                              |              |              | 104.7        |       |       |       |        |
| 1,3,6-Trioxacyclooctane                                                            |              |              | 48.8         |       |       |       |        |
| 1,3,5-Trioxane                                                                     | 15.11        |              | 56.6         |       |       |       |        |
| Triphenylarsine                                                                    |              |              | 99.3         |       |       |       |        |
| Triphenylbismuthine                                                                |              |              | 110.9        |       |       |       |        |
| Triphenylborane                                                                    |              |              | 81.6         |       |       |       |        |
| Triphenylene                                                                       |              |              | 118.0        |       |       |       |        |

**TABLE 6.2** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of Organic Compounds (*Continued*)

| Substance                              | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$ |       |       |        |
|----------------------------------------|--------------|--------------|--------------|-------|-------|-------|--------|
|                                        |              |              |              | 400 K | 600 K | 800 K | 1000 K |
| Triphenylmethane                       |              |              | 100.0        |       |       |       |        |
| Triphenylphosphine                     |              |              | 96           |       |       |       |        |
| Triphenylstibine                       |              |              | 106.3        |       |       |       |        |
| Tripropoxyborane                       |              |              | 49.4         |       |       |       |        |
| Tris(diethylamino)phosphine            |              |              | 60.7         |       |       |       |        |
| Tris(trimethylsilyl)amine              |              |              | 54.4         |       |       |       |        |
| Tropolone                              |              |              | 83.7         |       |       |       |        |
| Undecane                               | 22.32        | 41.5         | 56.4         | 327.1 | 442.7 | 525.9 | 588.3  |
| $\Delta H_f = 6.9^{-36.6}$             |              |              |              |       |       |       |        |
| Undecanenitrile                        |              |              | 71.1         |       |       |       |        |
| Undecanoic acid                        | 25.9         |              | 121.3        |       |       |       |        |
| 1-Undecene, $\Delta H_f = 9.2^{-55.8}$ | 16.99        | 40.9         | 55.4         | 312.7 | 421.1 | 499.3 | 557.3  |
| Uracil                                 |              |              | 126.5        |       |       |       |        |
| Urea                                   | 15.1         | 87.9         |              |       |       |       |        |
| (-)-Valine                             |              |              | 162.8        |       |       |       |        |
| Vinyl acetate                          |              | 34.4         | 34.8         |       |       |       |        |
| Vinyl benzene                          |              |              | 39.6         |       |       |       |        |
| Vinylcyclohexane                       |              |              | 39.7         |       |       |       |        |
| 4-Vinyl-1-cyclohexene                  |              | 33.5         | 38.3         |       |       |       |        |
| 1,2-Xylene                             | 13.61        | 36.2         | 43.4         | 171.7 | 234.2 | 278.8 | 311.1  |
| 1,3-Xylene                             | 11.55        | 35.7         | 42.7         | 167.5 | 232.2 | 277.9 | 310.6  |
| 1,4-Xylene                             | 16.81        | 35.7         | 42.4         | 166.1 | 230.8 | 276.7 | 309.7  |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds

| Substance                             | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|---------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Actinium                              |                |                                              |                                              |                                                        |                                                          |
| Ac                                    | c              | 0                                            | 0                                            | 56.5                                                   | 27.2                                                     |
| Aluminum                              |                |                                              |                                              |                                                        |                                                          |
| Al                                    | c              | 0                                            | 0                                            | 28.30(10)                                              | 24.4                                                     |
|                                       | g              | 330.0(40)                                    | 289.4                                        | 164.554(4)                                             | 21.4                                                     |
| Al <sup>3+</sup> std. state           | aq             | -538.4(15)                                   | -485.3                                       | -325.(10)                                              |                                                          |
| Al <sub>3</sub> BeO <sub>10</sub>     | c              | -5624                                        | -5317                                        | 175.6                                                  | 265.19                                                   |
| Al(BH <sub>4</sub> ) <sub>3</sub>     | lq             | -16.3                                        | 145.0                                        | 289.1                                                  | 194.6                                                    |
| AlBr <sub>3</sub>                     | c              | -527.2                                       | -488.5                                       | 180.2                                                  | 100.58                                                   |
| std. state                            | aq             | -895                                         | -799                                         | -74.5                                                  |                                                          |
| Al <sub>4</sub> C <sub>3</sub>        | c              | -216                                         | -203                                         | 89                                                     |                                                          |
| Al(CH <sub>3</sub> ) <sub>3</sub>     | lq             | 136.4                                        | -10.0                                        | 209.4                                                  | 155.6                                                    |
| Al(OAc) <sub>3</sub>                  | c              | -1892.4                                      |                                              |                                                        |                                                          |
| AlCl <sub>3</sub>                     | c              | -704.2                                       | -628.8                                       | 109.29                                                 | 91.13                                                    |
| std. state                            | aq             | -1033                                        | -878                                         | -152.3                                                 |                                                          |
| AlCl <sub>3</sub> · 6H <sub>2</sub> O | c              | -2692                                        | -2269                                        | 377                                                    |                                                          |
| AlF <sub>3</sub>                      | c              | -1510.4(13)                                  | -1431.1                                      | 66.5(5)                                                | 75.13                                                    |
| std. state                            | aq             | -1531.0                                      | -1322                                        | -363.2                                                 |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                    | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| AlF <sub>3</sub> · H <sub>2</sub> O                          | c              | -2297                                        | -2052                                        | 209                                                    |                                                          |
| AlH <sub>3</sub>                                             | c              | -46.0                                        |                                              | 30.0                                                   | 40.2                                                     |
| AlI <sub>3</sub>                                             | c              | -313.8                                       | -300.8                                       | 159.0                                                  | 98.7                                                     |
| std. state                                                   | aq             | -699                                         | -640                                         | 12.1                                                   |                                                          |
| AlK(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O      | c              | -6061.8                                      | -5141.7                                      | 687.4                                                  | 651.0                                                    |
| AlN                                                          | c              | -318.1                                       | -287.0                                       | 20.14                                                  | 30.10                                                    |
| Al(NO <sub>3</sub> ) <sub>3</sub> std. state                 | aq             | -1155                                        | -820                                         | 117.6                                                  |                                                          |
| Al(NO <sub>3</sub> ) <sub>3</sub> · 6H <sub>2</sub> O        | c              | -2850.5                                      | -2203.9                                      | 467.8                                                  | 433.0                                                    |
| Al(NO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O        | c              | -3757.1                                      | -2929.6                                      | 569                                                    |                                                          |
| AlO <sub>2</sub> <sup>-</sup> std. state                     | aq             | -930.9                                       | -830.9                                       | -36.8                                                  |                                                          |
| Al <sub>2</sub> O <sub>3</sub> corundum                      | c              | -1675.7(13)                                  | -1582.3                                      | 50.92(10)                                              | 79.15                                                    |
| Al(OH) <sub>3</sub>                                          | c              | -1284                                        | -1306                                        | 71                                                     | 93.1                                                     |
| Al(OH) <sub>3</sub> <sup>-</sup> std. state                  | aq             | -1502.5                                      | -1305.3                                      | 102.9                                                  |                                                          |
| AlP                                                          | c              | -166.5                                       |                                              |                                                        |                                                          |
| AlPO <sub>4</sub> berlinite                                  | c              | -1733.8                                      | -1618.0                                      | 90.79                                                  | 93.18                                                    |
| Al <sub>2</sub> S <sub>3</sub>                               | c              | -724.0                                       | -640                                         | 116.85                                                 | 105.06                                                   |
| Al <sub>2</sub> Se <sub>3</sub>                              | c              | -565                                         |                                              |                                                        |                                                          |
| Al <sub>2</sub> SiO <sub>5</sub> andalusite                  | c              | -2592.0                                      | -2444.8                                      | 93.2                                                   | 122.76                                                   |
| Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>              | c              | -3435                                        | -3507                                        | 239.3                                                  | 259.4                                                    |
| std. state                                                   | aq             | -3790                                        | -3205                                        | -583.3                                                 |                                                          |
| Al <sub>2</sub> Te <sub>3</sub>                              | c              | -326                                         |                                              |                                                        |                                                          |
| Americium                                                    |                |                                              |                                              |                                                        |                                                          |
| Am                                                           | c              | 0                                            | 0                                            | 62.7                                                   |                                                          |
| Am <sup>3+</sup>                                             | aq             | -682.8                                       | -671.5                                       | -159.0                                                 |                                                          |
| Am <sup>4+</sup>                                             | aq             | -511.7                                       | -461.1                                       | -372                                                   |                                                          |
| Am <sub>2</sub> O <sub>3</sub>                               | c              | -1757                                        | -1678                                        | 154.7                                                  |                                                          |
| AmO <sub>2</sub>                                             | c              | -1005.0                                      | 950.2                                        | 96.2                                                   |                                                          |
| Ammonium                                                     |                |                                              |                                              |                                                        |                                                          |
| NH <sub>3</sub>                                              | g              | -45.94(35)                                   | -16.4                                        | 192.776(5)                                             | 35.65                                                    |
| undissoc; std. state                                         | aq             | -80.29                                       | -26.57                                       | 111.3                                                  |                                                          |
| ND <sub>3</sub>                                              | g              | -58.6                                        | -26.0                                        | 203.9                                                  | 38.23                                                    |
| NH <sub>4</sub> <sup>+</sup> std. state                      | aq             | -133.26(25)                                  | -79.37                                       | 111.17(40)                                             | 79.9                                                     |
| NH <sub>4</sub> OH undissoc;<br>std. state                   | aq             | -361.2                                       | -254.0                                       | 165.5                                                  |                                                          |
| ionized; std. state                                          | aq             | -362.50                                      | -236.65                                      | 102.5                                                  | -68.6                                                    |
| NH <sub>4</sub> OAc                                          | c              | -616.14                                      |                                              |                                                        |                                                          |
| std. state                                                   | aq             | -618.52                                      | -448.78                                      | 200.0                                                  | 73.6                                                     |
| NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub>            | c              | -2352.2                                      | -2038.4                                      | 216.3                                                  | 226.44                                                   |
| std. state                                                   | aq             | -2481                                        | -2054                                        | -168.2                                                 |                                                          |
| NH <sub>4</sub> AsO <sub>2</sub> std. state                  | aq             | -561.54                                      | -429.41                                      | 154.8                                                  |                                                          |
| NH <sub>4</sub> H <sub>2</sub> AsO <sub>3</sub> std. state   | c              | -847.30                                      | -666.60                                      | 223.8                                                  |                                                          |
| NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>              | c              | -1059.8                                      | -833.0                                       | 172.05                                                 | 151.17                                                   |
| std. state                                                   | aq             | -1042.07                                     | -832.66                                      | 230.5                                                  |                                                          |
| (NH <sub>4</sub> ) <sub>2</sub> HAsO <sub>4</sub> std. state | aq             | -1171.1                                      | -873.20                                      | 225.1                                                  |                                                          |
| (NH <sub>4</sub> ) <sub>3</sub> AsO <sub>4</sub> std. state  | aq             | -1286.7                                      | -886.63                                      | 177.4                                                  |                                                          |
| NH <sub>4</sub> Br                                           | c              | -271.8                                       | -175.2                                       | 113.0                                                  | 96.0                                                     |
| std. state                                                   | aq             | -254.05                                      | -183.34                                      | 194.97                                                 | -61.9                                                    |
| NH <sub>4</sub> BrO <sub>3</sub>                             | aq             | -199.58                                      | -60.84                                       | 275.10                                                 |                                                          |
| NH <sub>4</sub> carbamate                                    | c              | -657.60                                      | -448.07                                      | 133.5                                                  |                                                          |
| NH <sub>4</sub> Cl                                           | c              | -314.5                                       | -202.9                                       | 94.6                                                   | 84.1                                                     |
| std. state                                                   | aq             | -299.66                                      | -210.62                                      | 169.9                                                  | -56.5                                                    |
| NH <sub>4</sub> ClO <sub>3</sub> std. state                  | aq             | -236.48                                      | -87.40                                       | 275.7                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                        | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|--------------------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| $\text{NH}_4\text{ClO}_4$                        | c              | −295.3                                                  | −88.8                                                   | 186.2                                                               | 128.1                                                                 |
| std. state                                       | aq             | −261.84                                                 | −87.99                                                  | 295.4                                                               |                                                                       |
| $\text{NH}_4\text{CN}$                           | c              | 0.4                                                     |                                                         |                                                                     | 134.0                                                                 |
| std. state                                       | aq             | 18.0                                                    | 92.9                                                    | 207.5                                                               |                                                                       |
| $\text{NH}_4\text{CNO}$ cyanate                  | aq             | −278.7                                                  | −177.0                                                  | 220.1                                                               |                                                                       |
| std. state                                       |                |                                                         |                                                         |                                                                     |                                                                       |
| $(\text{NH}_4)_2\text{CO}_3$ std. state          | aq             | −942.15                                                 | −686.64                                                 | 169.9                                                               |                                                                       |
| $(\text{NH}_4)_2\text{C}_2\text{O}_4$ oxalate    | c              | −1123.0                                                 |                                                         |                                                                     | 226.0                                                                 |
| $(\text{NH}_4)_2\text{CrO}_4$                    | c              | −1167.3                                                 |                                                         |                                                                     |                                                                       |
| std. state                                       | aq             | −1144.3                                                 | −886.59                                                 | 277.0                                                               |                                                                       |
| $(\text{NH}_4)_2\text{Cr}_2\text{O}_7$           | aq             | −1755.2                                                 | −1459.5                                                 | 488.7                                                               |                                                                       |
| $\text{NH}_4$ dithiocarbonate                    | c              | −126.8                                                  |                                                         |                                                                     |                                                                       |
| $\text{NH}_4\text{F}$                            | c              | −463.96                                                 | −348.78                                                 | 71.97                                                               | 65.27                                                                 |
| std. state                                       | aq             | −465.14                                                 | −358.19                                                 | 99.6                                                                | −26.8                                                                 |
| $\text{NH}_4$ formate std. state                 | aq             | −558.06                                                 | −430.5                                                  | 205.0                                                               | −7.9                                                                  |
| $\text{NH}_4\text{HCO}_3$                        | c              | −849.4                                                  | −665.9                                                  | 120.9                                                               |                                                                       |
|                                                  | aq             | −824.5                                                  | −666.1                                                  | 204.6                                                               |                                                                       |
| $\text{NH}_4\text{I}$                            | c              | −201.4                                                  | −112.5                                                  | 117.0                                                               | 81.8                                                                  |
| std. state                                       | aq             | −187.69                                                 | −130.96                                                 | 224.7                                                               | −62.3                                                                 |
| $\text{NH}_4\text{IO}_3$                         | c              | −385.8                                                  |                                                         |                                                                     |                                                                       |
| std. state                                       | aq             | −354.0                                                  | −207.5                                                  | 231.8                                                               |                                                                       |
| $\text{NH}_4\text{N}_3$ azide                    | c              | 115.5                                                   | 274.1                                                   | 112.6                                                               |                                                                       |
|                                                  | aq             | 142.7                                                   | 268.6                                                   | 221.3                                                               |                                                                       |
| $\text{NH}_4\text{NO}_2$                         | aq             | −237.2                                                  | −111.6                                                  | 236.4                                                               | −17.6                                                                 |
| $\text{NH}_4\text{NO}_3$                         | c              | −365.56                                                 | −184.01                                                 | 151.08                                                              | 139.3                                                                 |
| std. state                                       | aq             | −339.87                                                 | −190.71                                                 | 259.8                                                               | −6.7                                                                  |
| $\text{NH}_4\text{H}_2\text{PO}_4$               | c              | −1145.07                                                | −1210.56                                                | 151.96                                                              | 142.26                                                                |
| std. state                                       | aq             | −1428.79                                                | −1209.76                                                | 203.8                                                               |                                                                       |
| $(\text{NH}_4)_2\text{HPO}_4$                    | c              | −1556.91                                                |                                                         | 188.0                                                               |                                                                       |
| std. state                                       | aq             | −1557.16                                                | −1248.00                                                | 193.3                                                               |                                                                       |
| $\text{NH}_4\text{H}_3\text{P}_2\text{O}_7$      | aq             | −2409.1                                                 | −2102.6                                                 | 326.0                                                               |                                                                       |
| $\text{NH}_4\text{HS}$                           | c              | −156.9                                                  | −50.6                                                   | 97.5                                                                |                                                                       |
|                                                  | aq             | −150.2                                                  | −67.2                                                   | 176.1                                                               |                                                                       |
| $\text{NH}_4\text{HSO}_3$                        | aq             | −758.7                                                  | −607.0                                                  | 253.1                                                               |                                                                       |
| $\text{NH}_4\text{HSO}_4$                        | c              | −1026.96                                                |                                                         |                                                                     |                                                                       |
| std. state                                       | aq             | −1019.85                                                | −835.38                                                 | 245.2                                                               | −3.8                                                                  |
| $(\text{NH}_4)_3\text{PO}_4$                     | c              | −1671.9                                                 |                                                         |                                                                     |                                                                       |
| std. state                                       | aq             | −1674.9                                                 | −1256.9                                                 | 117                                                                 |                                                                       |
| $(\text{NH}_4)_4\text{P}_2\text{O}_7$ std. state | aq             | −2801.2                                                 | −2236.8                                                 | 335                                                                 |                                                                       |
| $(\text{NH}_4)_2\text{PtCl}_6$                   | c              | −803.3                                                  |                                                         |                                                                     | 237.7                                                                 |
| $\text{NH}_4\text{ReO}_4$                        | c              | −945.6                                                  | −774.9                                                  | 232.6                                                               |                                                                       |
| $(\text{NH}_4)_2\text{S}$                        | aq             | −231.8                                                  | −72.8                                                   | 212.1                                                               |                                                                       |
| $\text{NH}_4\text{SCN}$                          | aq             | −56.1                                                   | 13.4                                                    | 257.7                                                               | 39.7                                                                  |
| $\text{NH}_4\text{HSeO}_4$ std. state            | aq             | −714.2                                                  | −531.6                                                  | 262.8                                                               |                                                                       |
| $(\text{NH}_4)_2\text{SeO}_4$                    | aq             | −864.0                                                  | −599.8                                                  | 280.7                                                               |                                                                       |
| $(\text{NH}_4)_2\text{SiF}_6$                    | c              | −2681.69                                                | −2365.3                                                 | 280.24                                                              | 228.11                                                                |
| $(\text{NH}_4)_2\text{SO}_3$                     | aq             | −900.4                                                  | −645.0                                                  | 197.5                                                               |                                                                       |
| $(\text{NH}_4)_2\text{SO}_4$                     | c              | −1180.9                                                 | −901.70                                                 | 220.1                                                               | 187.49                                                                |
| std. state                                       | aq             | −1174.28                                                | −903.37                                                 | 246.9                                                               | −133.1                                                                |
| $(\text{NH}_4)_2\text{S}_2\text{O}_8$            | c              | −1648.08                                                |                                                         |                                                                     |                                                                       |
| std. state                                       | aq             | −1610.0                                                 | −1273.6                                                 | 471.1                                                               |                                                                       |
| $\text{NH}_4\text{VO}_3$                         | c              | −1053.1                                                 | −888.3                                                  | 140.6                                                               | 129.33                                                                |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                             | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|-------------------------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| Antimony                                              |                |                                                         |                                                         |                                                                     |                                                                       |
| Sb                                                    | c              | 0                                                       | 0                                                       | 45.7                                                                | 25.2                                                                  |
|                                                       | g              | 262.3                                                   | 222.1                                                   | 180.3                                                               | 20.8                                                                  |
| SbBr <sub>3</sub>                                     | c              | −259.4                                                  | −239.3                                                  | 207.1                                                               |                                                                       |
|                                                       | g              | −194.6                                                  | −223.9                                                  | 372.9                                                               | 80.2                                                                  |
| SbCl <sub>3</sub>                                     | c              | −382.0                                                  | −323.7                                                  | 184.1                                                               | 107.9                                                                 |
| SbCl <sub>5</sub>                                     | lq             | −440.16                                                 | −350.2                                                  | 301                                                                 |                                                                       |
| SbF <sub>3</sub>                                      | c              | −915.5                                                  |                                                         |                                                                     |                                                                       |
| SbH <sub>3</sub>                                      | g              | 145.11                                                  | 147.74                                                  | 232.8                                                               | 41.05                                                                 |
| SbI <sub>3</sub>                                      | c              | −100.4                                                  |                                                         | 215.5                                                               | 97.57                                                                 |
| Sb <sub>2</sub> O <sub>3</sub>                        | c              | −708.8                                                  |                                                         | 123.01                                                              | 101.25                                                                |
| Sb <sub>2</sub> O <sub>5</sub>                        | c              | −971.9                                                  | −829.2                                                  | 125.1                                                               | 117.61                                                                |
| Sb <sub>2</sub> S <sub>3</sub>                        | c              | −174.9                                                  |                                                         | 182.0                                                               | 117.74                                                                |
| Sb <sub>2</sub> Te <sub>3</sub>                       | c              | −56.5                                                   | −55.2                                                   | 234                                                                 |                                                                       |
| Argon                                                 |                |                                                         |                                                         |                                                                     |                                                                       |
| Ar                                                    | g              | 0                                                       | 0                                                       | 154.846(3)                                                          | 20.79                                                                 |
| Arsenic                                               |                |                                                         |                                                         |                                                                     |                                                                       |
| As gray                                               | c              | 0                                                       | 0                                                       | 35.1                                                                | 24.64                                                                 |
| AsBr <sub>3</sub>                                     | g              | −130.0                                                  | −159.0                                                  | 363.9                                                               | 79.16                                                                 |
| AsCl <sub>3</sub>                                     | lq             | −305.0                                                  | −259.4                                                  | 216.3                                                               | 133.5                                                                 |
|                                                       | g              | −261.5                                                  | −248.9                                                  | 327.06                                                              | 75.73                                                                 |
| AsF <sub>3</sub>                                      | lq             | −821.3                                                  | −774.2                                                  | 181.2                                                               | 126.2                                                                 |
|                                                       | g              | −785.8                                                  | −770.8                                                  | 289.1                                                               | 65.6                                                                  |
| AsH <sub>3</sub>                                      | g              | 66.44                                                   | 68.91                                                   | 222.8                                                               | 38.07                                                                 |
| AsI <sub>3</sub>                                      | c              | −58.2                                                   | −59.4                                                   | 213.05                                                              | 105.77                                                                |
| AsO <sub>2</sub> <sup>−</sup>                         | aq             | −429.0                                                  | −350.0                                                  | 40.6                                                                |                                                                       |
| AsO <sub>4</sub> <sup>3−</sup>                        | aq             | −888.1                                                  | −648.4                                                  | −162.8                                                              |                                                                       |
| As <sub>2</sub> O <sub>5</sub>                        | c              | −924.87                                                 | −782.3                                                  | 105.4                                                               | 116.5                                                                 |
| As <sub>4</sub> O <sub>6</sub> octahedral             | c              | −1313.94                                                | −1152.52                                                | 214.2                                                               | 191.29                                                                |
| As <sub>2</sub> S <sub>3</sub>                        | c              | −169.0                                                  | −168.6                                                  | 163.6                                                               | 116.3                                                                 |
| Astatine                                              |                |                                                         |                                                         |                                                                     |                                                                       |
| At                                                    | c              | 0                                                       | 0                                                       | 121.3                                                               |                                                                       |
| Barium                                                |                |                                                         |                                                         |                                                                     |                                                                       |
| Ba                                                    | c              | 0                                                       | 0                                                       | 62.48                                                               | 28.10                                                                 |
| Ba <sup>2+</sup> std. state                           | aq             | −537.64                                                 | −560.74                                                 | 9.6                                                                 |                                                                       |
| Ba(OAc) <sub>2</sub> acetate                          | c              | −1484.5                                                 |                                                         |                                                                     |                                                                       |
| std. state                                            | aq             | −1509.67                                                | −1299.55                                                | 182.8                                                               |                                                                       |
| BaBr <sub>2</sub>                                     | c              | −757.3                                                  | −736.8                                                  | 146.0                                                               | 77.0                                                                  |
| std. state                                            | aq             | −780.73                                                 | −768.68                                                 | 174.5                                                               |                                                                       |
| BaBr <sub>2</sub> · 2H <sub>2</sub> O                 | c              | −1366.1                                                 | −1230.5                                                 | 226                                                                 |                                                                       |
| Ba(BrO <sub>3</sub> ) <sub>2</sub>                    | c              | −752.66                                                 | −577.4                                                  | 243                                                                 |                                                                       |
| BaC <sub>2</sub> O <sub>4</sub> oxalate               | c              | −1368.6                                                 |                                                         |                                                                     |                                                                       |
| BaCl <sub>2</sub>                                     | c              | −855.0                                                  | −806.7                                                  | 123.67                                                              | 75.14                                                                 |
| BaCl <sub>2</sub> · 2H <sub>2</sub> O                 | c              | −1456.9                                                 | −1293.2                                                 | 202.9                                                               | 161.96                                                                |
| Ba(ClO <sub>3</sub> ) <sub>2</sub>                    | c              | −762.7                                                  |                                                         |                                                                     |                                                                       |
| Ba(ClO <sub>3</sub> ) <sub>2</sub> · H <sub>2</sub> O | c              | −1691.6                                                 | −1270.7                                                 | 393                                                                 |                                                                       |
| BaCO <sub>3</sub> witherite                           | c              | −1213.0                                                 | −1134.4                                                 | 112.1                                                               | 86.0                                                                  |
| BaCrO <sub>4</sub>                                    | c              | −1446.0                                                 | −1345.3                                                 | 158.6                                                               |                                                                       |
| BaF <sub>2</sub>                                      | c              | −1207.1                                                 | −1156.8                                                 | 96.4                                                                | 71.20                                                                 |
| std. state                                            | aq             | −1202.90                                                | −1118.38                                                | −17.0                                                               |                                                                       |
| Ba(HCO <sub>3</sub> ) <sub>2</sub> std. state         | aq             | −1921.63                                                | −1734.4                                                 | 192.1                                                               |                                                                       |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                        | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Ba(H <sub>2</sub> PO <sub>3</sub> ) <sub>2</sub> | c              | -1762.3                                      |                                              |                                                        |                                                          |
| BaI <sub>2</sub>                                 | c              | -602.1                                       | -601.4                                       | 165.1                                                  | 77.49                                                    |
| std. state                                       | aq             | -648.02                                      | -663.92                                      | 232.2                                                  |                                                          |
| Ba(IO <sub>3</sub> ) <sub>2</sub>                | c              | -1027.2                                      | -864.8                                       | 249.4                                                  | 187.4                                                    |
| std. state                                       | aq             | -980.3                                       | -816.7                                       | 246.4                                                  |                                                          |
| BaMnO <sub>4</sub>                               | c              | -1548                                        | -1439.7                                      | 138                                                    | 140.6                                                    |
| BaMoO <sub>4</sub>                               | c              | -1507.5                                      | -1439.7                                      | 144.3                                                  | 114.7                                                    |
| Ba(NO <sub>2</sub> ) <sub>2</sub>                | c              | -768.2                                       |                                              |                                                        |                                                          |
| Ba(NO <sub>3</sub> ) <sub>2</sub>                | c              | -988.0                                       | -792.6                                       | 213.8                                                  | 151.38                                                   |
| std. state                                       | aq             | -952.36                                      | -783.41                                      | 302.5                                                  |                                                          |
| BaO                                              | c              | -548.0                                       | -520.4                                       | 72.07                                                  | 47.28                                                    |
| BaO <sub>2</sub>                                 | c              | -634.3                                       |                                              |                                                        |                                                          |
| Ba(OH) <sub>2</sub>                              | c              | -944.7                                       | -859.5                                       | 107                                                    | 101.6                                                    |
| Ba(OH) <sub>2</sub> · H <sub>2</sub> O           | c              | -3342.2                                      | -2793.2                                      | 427                                                    |                                                          |
| BaS                                              | c              | -460.0                                       | -456.0                                       | 78.2                                                   | 49.37                                                    |
| BaSe                                             | c              | -372                                         |                                              |                                                        |                                                          |
| BaSeO <sub>3</sub>                               | c              | -1040.6                                      | -968.2                                       | 167                                                    |                                                          |
| BaSiF <sub>6</sub>                               | c              | -1952.2                                      | -2794.1                                      | 163                                                    |                                                          |
| BaSO <sub>3</sub>                                | c              | -1179.5                                      |                                              |                                                        |                                                          |
| BaSO <sub>4</sub>                                | c              | -1473.19                                     | -1362.2                                      | 132.2                                                  | 101.75                                                   |
| BaTiO <sub>3</sub>                               | c              | -1659.8                                      | -1572.4                                      | 108.0                                                  | 102.47                                                   |
| Beryllium                                        |                |                                              |                                              |                                                        |                                                          |
| Be                                               | c              | 0                                            | 0                                            | 9.50(8)                                                | 16.38                                                    |
|                                                  | g              | 324.(5)                                      |                                              | 136.275(3)                                             |                                                          |
| Be <sup>2+</sup> std. state                      | aq             | -382.8                                       | -379.7                                       | -129.7                                                 |                                                          |
| BeAl <sub>2</sub> O <sub>4</sub> chrysoberyl     | c              | -2301.0                                      | -2178.5                                      | 66.29                                                  | 105.38                                                   |
| BeBr <sub>2</sub>                                | c              | -353.5                                       | -337                                         | 108.0                                                  | 69.4                                                     |
| Be <sub>2</sub> C                                | c              | 91                                           | -88                                          | 16.3                                                   | 43.2                                                     |
| BeCl <sub>2</sub> β form                         | c              | -490.4                                       | -445.6                                       | 75.81                                                  | 62.43                                                    |
| BeCO <sub>3</sub>                                | c              | 1025.0                                       |                                              | 52.0                                                   | 65.0                                                     |
| BeF <sub>2</sub> α form                          | c              | -1026.8                                      | -979.4                                       | 53.35                                                  | 51.82                                                    |
| BeI <sub>2</sub>                                 | c              | -192.5                                       | -187                                         | 121.0                                                  | 71.1                                                     |
| Be <sub>3</sub> N <sub>2</sub> cubic             | c              | -588.3                                       | -532.9                                       | 34.13                                                  | 64.36                                                    |
| BeO α form                                       | c              | -609.4(25)                                   | -580.1                                       | 13.77(4)                                               | 25.56                                                    |
| BeO <sub>2</sub> <sup>-</sup>                    | aq             | -790.8                                       | -640.1                                       | -159.0                                                 |                                                          |
| 3BeO · B <sub>2</sub> O <sub>3</sub>             | c              | -3105                                        | -2939                                        | 100                                                    | 139.7                                                    |
| Be(OH) <sub>2</sub> β form                       | c              | -902.5                                       | -815.0                                       | 45.5                                                   | 62.1                                                     |
| BeS                                              | c              | -234.3                                       | -233.0                                       | 34.0                                                   | 34.0                                                     |
| BeSeO <sub>4</sub>                               | c              | -1205.2                                      | -1093.8                                      | 77.9                                                   | 85.7                                                     |
| std. state                                       | aq             | -982.0                                       | -820.9                                       | -75.7                                                  |                                                          |
| Be <sub>2</sub> SiO <sub>4</sub>                 | c              | -2117                                        | -2003                                        | 64.19                                                  | 95.6                                                     |
| BeSO <sub>4</sub>                                | c              | -1200.8                                      | -1089.4                                      | 77.97                                                  | 85.70                                                    |
| std. state                                       | aq             | -1290.0                                      | -1124.3                                      | -109.6                                                 |                                                          |
| BeSO <sub>4</sub> · H <sub>2</sub> O             | c              | -2423.75                                     | -2080.66                                     | 232.97                                                 | 216.61                                                   |
| BeWO <sub>4</sub>                                | c              | -1513                                        | -1405                                        | 88.4                                                   | 97.3                                                     |
| Bismuth                                          |                |                                              |                                              |                                                        |                                                          |
| Bi                                               | c              | 0                                            | 0                                            | 56.7                                                   | 25.5                                                     |
|                                                  | g              | 207.1                                        | 168.2                                        | 187.0                                                  | 20.8                                                     |
| BiBr <sub>3</sub>                                | c              | 264                                          | 234                                          | 226                                                    | 109                                                      |
| BiCl <sub>3</sub>                                | c              | -379.1                                       | -315.1                                       | 177.0                                                  | 105.0                                                    |
| BiH <sub>3</sub>                                 | g              | 277.8                                        |                                              |                                                        |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                             | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| BiI <sub>3</sub>                                      | c              | −100.4                                       | −175.3                                       |                                                        |                                                          |
| Bi <sub>2</sub> O <sub>3</sub>                        | c              | −574.0                                       | −493.7                                       | 151.5                                                  | 113.5                                                    |
| BiOCl                                                 | c              | −366.9                                       | −322.2                                       | 120.5                                                  |                                                          |
| Bi <sub>2</sub> S <sub>3</sub>                        | c              | −143.1                                       | −140.6                                       | 200.4                                                  | 122.2                                                    |
| Bi <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>       | c              | −2544.3                                      |                                              |                                                        |                                                          |
| Bi <sub>7</sub> Te <sub>3</sub>                       | c              | −78.24                                       |                                              | 260.91                                                 | 152.21                                                   |
| Boron                                                 |                |                                              |                                              |                                                        |                                                          |
| B                                                     | c              | 0                                            | 0                                            | 5.90(8)                                                | 11.1                                                     |
|                                                       | g              | 565.(5)                                      |                                              | 153.436(15)                                            |                                                          |
| BBr <sub>3</sub>                                      | lq             | −239.7                                       | −238.5                                       | 229.7                                                  | 128.03                                                   |
| B <sub>4</sub> C                                      | c              | −62.7                                        | −62.1                                        | 27.18                                                  | 53.76                                                    |
| BCl <sub>3</sub>                                      | g              | −403.8                                       | −388.7                                       | 290.1                                                  | 62.7                                                     |
| BF <sub>3</sub>                                       | g              | −1136.0(8)                                   | −1119.4                                      | 254.42(20)                                             | 50.45                                                    |
| BF <sub>4</sub> <sup>−</sup> std. state               | aq             | −1574.9                                      | −1487.0                                      | 179.9                                                  |                                                          |
| BH <sub>3</sub>                                       | g              | 100.0                                        | 111                                          | 187.9                                                  | 36.22                                                    |
| BH <sub>4</sub> <sup>−</sup> std. state               | aq             | 48.16                                        | 114.27                                       | 110.5                                                  |                                                          |
| B <sub>2</sub> H <sub>6</sub> diborane(6)             | g              | 35.6                                         | 86.7                                         | 232.1                                                  | 56.9                                                     |
| B <sub>3</sub> H <sub>9</sub> pentaborane(9)          | lq             | 42.7                                         | 171.8                                        | 184.2                                                  | 151.13                                                   |
| B <sub>10</sub> H <sub>14</sub> decaborane(14)        | c              | −29.83                                       | 212.9                                        | 234.9                                                  | 221.2                                                    |
| BN                                                    | c              | −254.4                                       | −228.4                                       | 14.80                                                  | 19.72                                                    |
| B <sub>3</sub> N <sub>3</sub> H <sub>6</sub> borazine | lq             | −541.0                                       | −392.7                                       | 199.6                                                  |                                                          |
|                                                       | g              | −510                                         | −389                                         | 288.61                                                 | 96.94                                                    |
| BO <sub>2</sub> <sup>−</sup> std. state               | aq             | −772.37                                      | −678.94                                      | −37.24                                                 |                                                          |
| B <sub>2</sub> O <sub>3</sub>                         | c              | −1273.5(14)                                  | −1194.3                                      | 53.97(30)                                              | 62.8                                                     |
| B(OH) <sub>4</sub> <sup>−</sup> std. state            | aq             | −1344.03                                     | −1153.32                                     | 102.5                                                  |                                                          |
| B <sub>3</sub> O <sub>3</sub> H <sub>3</sub> boroxin  | c              | −1262                                        | −11.56                                       | 167                                                    | 98.3                                                     |
| B <sub>2</sub> S <sub>3</sub>                         | c              | −240.6                                       |                                              | 100.0                                                  | 111.7                                                    |
| Bromine                                               |                |                                              |                                              |                                                        |                                                          |
| Br atomic                                             | g              | 111.87(12)                                   | 82.4                                         | 175.018(4)                                             | 20.8                                                     |
| Br <sup>−</sup> std. state                            | aq             | −121.41(15)                                  | −103.97                                      | 82.55(20)                                              | −141.8                                                   |
| Br <sub>2</sub>                                       | lq             | 0                                            | 0                                            | 152.21(30)                                             | 75.67                                                    |
|                                                       | g              | 30.91(11)                                    |                                              | 245.468(5)                                             |                                                          |
| Br <sub>3</sub> <sup>−</sup> std. state               | aq             | −130.42                                      | −107.07                                      | 215.5                                                  |                                                          |
| BrCl                                                  | g              | 14.6                                         | −0.96                                        | 239.91                                                 | 34.98                                                    |
| BrF                                                   | g              | −93.8                                        | −109.2                                       | 229.0                                                  | 32.97                                                    |
| BrF <sub>3</sub>                                      | lq             | −300.8                                       | −240.5                                       | 178.2                                                  | 124.6                                                    |
|                                                       | g              | −255.6                                       | 229.4                                        | 292.5                                                  | 66.6                                                     |
| BrF <sub>5</sub>                                      | lq             | −458.6                                       | −351.9                                       | 225.1                                                  |                                                          |
|                                                       | g              | −428.9                                       | −351.6                                       | 323.2                                                  | 99.6                                                     |
| BrO <sup>−</sup> std. state                           | aq             | −94.1                                        | −33.5                                        | 42.0                                                   |                                                          |
| BrO <sub>2</sub> <sup>−</sup> std. state              | aq             | −67.07                                       | 18.6                                         | 161.71                                                 |                                                          |
| BrO <sub>4</sub> <sup>−</sup>                         | aq             | 13.0                                         | 118.1                                        | 199.6                                                  |                                                          |
| Cadmium                                               |                |                                              |                                              |                                                        |                                                          |
| Cd                                                    | c              | 0                                            | 0                                            | 51.80(15)                                              | 25.9                                                     |
|                                                       | g              | 111.80(20)                                   |                                              | 167.749(4)                                             | 20.8                                                     |
| Cd <sup>2+</sup>                                      | aq             | −75.92(60)                                   |                                              | −72.8(15)                                              |                                                          |
| CdBr <sub>2</sub>                                     | c              | −316.18                                      | −296.31                                      | 137.2                                                  | 76.7                                                     |
| std. state                                            | aq             | −318.99                                      | −285.52                                      | 91.6                                                   |                                                          |
| CdCl <sub>2</sub>                                     | c              | −391.6                                       | −343.9                                       | 115.3                                                  | 74.7                                                     |
| std. state                                            | aq             | −410.20                                      | −340.12                                      | 39.8                                                   |                                                          |
| CdCl <sub>2</sub> · 5/2H <sub>2</sub> O               | c              | −1131.94                                     | −944.08                                      | 227.2                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                      | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Cd(CN) <sub>2</sub>                                            | c              | 162.3                                        |                                              |                                                        |                                                          |
| std. state                                                     | aq             | 225.5                                        | 267.4                                        | 115.1                                                  |                                                          |
| CdCO <sub>3</sub>                                              | c              | -750.6                                       | -669.4                                       | 92.5                                                   |                                                          |
| Cd(OAc) <sub>2</sub> std. state                                | aq             | -1047.9                                      | -816.4                                       | 100                                                    |                                                          |
| CdF <sub>2</sub>                                               | c              | -700.4                                       | -647.7                                       | 77.4                                                   |                                                          |
| std. state                                                     | aq             | -741.15                                      | -635.21                                      | -100.8                                                 |                                                          |
| CdI <sub>2</sub>                                               | c              | -203.3                                       | -201.4                                       | 161.1                                                  | 80.0                                                     |
| std. state                                                     | aq             | -186.3                                       | -180.8                                       | 149.4                                                  |                                                          |
| CdI <sub>4</sub> std. state                                    | aq             | -341.8                                       | -315.9                                       | 326                                                    |                                                          |
| Cd(NH <sub>3</sub> ) <sub>4</sub> <sup>2+</sup> std. state     | aq             | -450.2                                       | -226.4                                       | 336.4                                                  |                                                          |
| Cd(NO <sub>3</sub> ) <sub>2</sub>                              | c              | -456.3                                       |                                              |                                                        |                                                          |
| std. state                                                     | aq             | -490.6                                       | -300.2                                       | 219.7                                                  |                                                          |
| CdO                                                            | c              | -258.35(40)                                  | -228.7                                       | 54.8(15)                                               | 43.4                                                     |
| Cd(OH) <sub>2</sub>                                            | c              | -560.7                                       | -473.6                                       | 96.0                                                   |                                                          |
| CdS                                                            | c              | -161.9                                       | -156.5                                       | 64.9                                                   | 55.5                                                     |
| CdSO <sub>4</sub>                                              | c              | -933.4                                       | -822.7                                       | 123.0                                                  | 99.6                                                     |
| std. state                                                     | aq             | -985.2                                       | -822.2                                       | -53.1                                                  |                                                          |
| CdSO <sub>4</sub> · 8/3H <sub>2</sub> O                        | c              | -1729.30(80)                                 | -1465.3                                      | 229.65(40)                                             | 213.3                                                    |
| CdSeO <sub>4</sub>                                             | c              | -633.0                                       | -531.8                                       | 164.4                                                  |                                                          |
| std. state                                                     | aq             | -674.9                                       | -518.8                                       | -19.3                                                  |                                                          |
| CdTe                                                           | c              | -92.5                                        | -92.0                                        | 100.0                                                  |                                                          |
| Calcium                                                        |                |                                              |                                              |                                                        |                                                          |
| Ca                                                             | c              | 0                                            | 0                                            | 41.59(40)                                              | 25.9                                                     |
|                                                                | g              | 177.8(8)                                     |                                              | 154.887(4)                                             |                                                          |
| Ca <sup>2+</sup> std. state                                    | aq             | -543.0(10)                                   | -553.54                                      | -56.2(10)                                              |                                                          |
| Ca(OAc) <sub>2</sub>                                           | c              | -1479.5                                      |                                              |                                                        |                                                          |
| std. state                                                     | aq             | -1514.73                                     | -1292.35                                     | 120.1                                                  |                                                          |
| Ca <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>               | c              | -3298.7                                      | -3063.1                                      | 226                                                    |                                                          |
| Ca(BO <sub>2</sub> ) <sub>2</sub>                              | c              | -2030.9                                      | -1924.1                                      | 104.85                                                 | 103.98                                                   |
| CaB <sub>4</sub> O <sub>7</sub>                                | c              | -3360.3                                      | -3167.1                                      | 134.7                                                  | 157.9                                                    |
| CaBr <sub>2</sub>                                              | c              | -682.8                                       | -663.6                                       | 130.0                                                  | 75.04                                                    |
| std. state                                                     | aq             | -785.9                                       | -761.5                                       | 111.7                                                  |                                                          |
| CaC <sub>2</sub>                                               | c              | -59.8                                        | -64.9                                        | 69.96                                                  | 62.72                                                    |
| CaCl <sub>2</sub>                                              | c              | -795.4                                       | -748.8                                       | 108.4                                                  | 72.9                                                     |
| std. state                                                     | aq             | -877.13                                      | -816.05                                      | 59.8                                                   |                                                          |
| CaCl <sub>2</sub> · 2H <sub>2</sub> O                          | c              | -1402.9                                      |                                              |                                                        | 738                                                      |
| CaCN <sub>2</sub> cyanamide                                    | c              | -350.6                                       |                                              |                                                        |                                                          |
| Ca(CN) <sub>2</sub>                                            | c              | -184.5                                       |                                              |                                                        |                                                          |
| CaCO <sub>3</sub> calcite                                      | c              | -1207.6                                      | -1129.1                                      | 91.7                                                   | 83.5                                                     |
| aragonite                                                      | c              | -1207.8                                      | -1128.2                                      | 88.0                                                   | 82.3                                                     |
|                                                                | aq             | -1220.0                                      | -1081.4                                      | -110.0                                                 |                                                          |
| CaC <sub>2</sub> O <sub>4</sub>                                | c              | -1360.6                                      |                                              |                                                        |                                                          |
| CaC <sub>2</sub> O <sub>4</sub> · H <sub>2</sub> O             | c              | -1674.9                                      | -1514.0                                      | 156.5                                                  | 152.8                                                    |
| CaCrO <sub>4</sub>                                             | c              | -1379.1                                      | -1277.4                                      | 134                                                    |                                                          |
| CaF <sub>2</sub>                                               | c              | -1228.0                                      | -1175.6                                      | 68.6                                                   | 67.0                                                     |
|                                                                | aq             | -1208.1                                      | -1111.2                                      | -80.8                                                  |                                                          |
| Ca(formate) <sub>2</sub>                                       | c              | 1386.6                                       |                                              |                                                        |                                                          |
| CaH <sub>2</sub>                                               | c              | -181.5                                       | -142.5                                       | 41.4                                                   | 41.0                                                     |
| CaHPO <sub>4</sub> · 2H <sub>2</sub> O                         | c              | -2403.58                                     | -2154.75                                     | 189.45                                                 | 197.07                                                   |
| Ca(H <sub>2</sub> PO <sub>2</sub> ) <sub>2</sub> hypophosphite | c              | -1752.7                                      |                                              |                                                        |                                                          |
| Ca(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> std. state    | aq             | -3135.41                                     | -2814.33                                     | 127.6                                                  |                                                          |



**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                        | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Ca(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> · H <sub>2</sub> O              | c              | − 3409.67                                    | − 3058.42                                    | 259.8                                                  | 258.82                                                   |
| CaI <sub>2</sub>                                                                 | c              | − 533.5                                      | − 528.9                                      | 142.0                                                  | 77.16                                                    |
| std. state                                                                       | aq             | − 653.2                                      | − 656.7                                      | 169.5                                                  |                                                          |
| Ca(IO <sub>3</sub> ) <sub>2</sub>                                                | c              | − 1002.5                                     | − 839.3                                      | 230                                                    |                                                          |
| Ca[Mg(CO <sub>3</sub> ) <sub>2</sub> ] dolomite                                  | c              | − 2326.3                                     | − 2163.6                                     | 155.18                                                 | 157.53                                                   |
| CaMoO <sub>4</sub>                                                               | c              | − 1541.4                                     | − 1434.7                                     | 122.6                                                  | 114.3                                                    |
| Ca <sub>3</sub> N <sub>2</sub>                                                   | c              | − 439.3                                      |                                              | 105.0                                                  | 113.0                                                    |
| Ca(NO <sub>2</sub> ) <sub>2</sub>                                                | c              | − 741.4                                      |                                              |                                                        |                                                          |
| Ca(NO <sub>3</sub> ) <sub>2</sub>                                                | c              | − 938.2                                      | − 742.8                                      | 193.3                                                  | 149.37                                                   |
| std. state                                                                       | aq             | − 957.55                                     | − 776.22                                     | 239.7                                                  |                                                          |
| CaO                                                                              | c              | − 634.92(90)                                 | − 603.3                                      | 38.1(4)                                                | 42.0                                                     |
| Ca(OH) <sub>2</sub>                                                              | c              | − 985.2                                      | − 897.5                                      | 83.4                                                   | 87.5                                                     |
| Ca <sub>3</sub> P <sub>2</sub>                                                   | c              | − 506                                        |                                              |                                                        |                                                          |
| Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>                                  | c              | − 4120.8                                     | − 3884.8                                     | 236.0                                                  | 227.8                                                    |
| Ca <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                                    | c              | − 3338.8                                     | − 3132.1                                     | 189.24                                                 | 187.8                                                    |
| Ca <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub><br>fluoroapatite | c              | − 13,744                                     | − 12,983                                     | 775.7                                                  | 751.9                                                    |
| CaS                                                                              | c              | − 482.4                                      | − 477.4                                      | 56.5                                                   | 47.4                                                     |
| CaSe                                                                             | c              | − 368.2                                      | − 363.2                                      | 67                                                     |                                                          |
| CaSiO <sub>3</sub>                                                               | c              | − 1634.9                                     | − 1549.7                                     | 81.92                                                  | 85.27                                                    |
| Ca <sub>2</sub> SiO <sub>4</sub>                                                 | c              | − 2307.5                                     | − 2192.8                                     | 127.7                                                  | 128.8                                                    |
| 3CaO · SiO <sub>2</sub>                                                          | c              | − 2929.2                                     | − 2784.0                                     | 168.6                                                  | 171.9                                                    |
| CaSO <sub>3</sub> · 2H <sub>2</sub> O                                            | c              | − 1752.7                                     | − 1555.2                                     | 184                                                    | 178.7                                                    |
| CaSO <sub>4</sub>                                                                | c              | − 1425.2                                     | − 1309.1                                     | 108.4                                                  | 99.0                                                     |
|                                                                                  | aq             | − 1451.1                                     | − 1298.1                                     | − 33.1                                                 |                                                          |
| CaSO <sub>4</sub> · ½H <sub>2</sub> O                                            | c              | − 1576.7                                     | − 1436.8                                     | 130.5                                                  | 119.4                                                    |
| CaSO <sub>4</sub> · 2H <sub>2</sub> O                                            | c              | − 2022.6                                     | − 1797.5                                     | 194.1                                                  | 186.0                                                    |
| Ca(VO <sub>3</sub> ) <sub>2</sub>                                                | c              | − 2329.3                                     | − 2169.7                                     | 179.1                                                  | 166.8                                                    |
| CaWO <sub>4</sub>                                                                | c              | − 1645.15                                    | − 1538.50                                    | 126.40                                                 | 114.14                                                   |
| Carbon                                                                           |                |                                              |                                              |                                                        |                                                          |
| C graphite                                                                       | c              | 0                                            | 0                                            | 5.74(10)                                               | 8.517                                                    |
|                                                                                  | g              | 716.68(45)                                   |                                              | 158.100(3)                                             |                                                          |
| diamond                                                                          | c              | 1.897                                        | 2.900                                        | 2.377                                                  | 6.116                                                    |
| CN <sup>−</sup>                                                                  | aq             | 150.6                                        | 172.4                                        | 94.1                                                   |                                                          |
| (CN) <sub>2</sub> cyanogen                                                       | g              | 306.7                                        | 297.2                                        | 241.9                                                  | 56.9                                                     |
| CNBr                                                                             | g              | 186.2                                        | 165.3                                        | 248.36                                                 | 46.9                                                     |
| CNCl                                                                             | g              | 137.95                                       | 131.02                                       | 236.2                                                  | 45.0                                                     |
| CNF                                                                              | g              |                                              |                                              | 224.7                                                  | 41.8                                                     |
| CNI                                                                              | c              | 166.2                                        | 185.0                                        | 96.2                                                   |                                                          |
|                                                                                  | g              | 225.5                                        | 196.6                                        | 256.8                                                  | 48.3                                                     |
| CNN <sub>3</sub> cyanogen azide                                                  | c              | 387.4                                        |                                              |                                                        |                                                          |
| OCN <sup>−</sup>                                                                 | aq             | − 146.0                                      | − 97.4                                       | 106.7                                                  |                                                          |
| CO                                                                               | g              | − 110.53(17)                                 | − 137.16                                     | 197.660(4)                                             | 29.14                                                    |
| CO <sub>2</sub>                                                                  | g              | − 393.51(13)                                 | 394.39                                       | 213.785(10)                                            | 37.13                                                    |
| undissoc; std. state                                                             | aq             | − 413.26(20)                                 | − 386.0                                      | 119.36(60)                                             |                                                          |
| CO <sub>3</sub> <sup>2−</sup>                                                    | aq             | − 675.23(25)                                 | − 527.9                                      | − 50.0(10)                                             |                                                          |
| C <sub>3</sub> O <sub>2</sub> suboxide                                           | g              | − 93.7                                       | − 109.8                                      | 276.4                                                  | 67.0                                                     |
| COBr <sub>2</sub>                                                                | g              | − 96.2                                       | − 110.9                                      | 309.1                                                  | 61.8                                                     |
| COCl <sub>2</sub> phosgene                                                       | g              | − 219.1                                      | − 204.9                                      | 283.50                                                 | 57.70                                                    |
| COClF                                                                            | g              |                                              |                                              | 276.7                                                  | 52.4                                                     |
| COF <sub>2</sub>                                                                 | g              | − 639.8                                      | − 623.33                                     | 258.89                                                 | 46.8                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                           | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|---------------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| COS carbonyl sulfide                                                | g              | -142.0                                       | -166.9                                       | 231.56                                                 | 41.50                                                    |
| CS <sub>2</sub>                                                     | lq             | 89.0                                         |                                              |                                                        | 74.6                                                     |
|                                                                     | g              | 117.7                                        | 67.1                                         | 237.8                                                  | 45.4                                                     |
| CTe <sub>2</sub>                                                    | lq             | 164.8                                        |                                              |                                                        |                                                          |
| Cerium                                                              |                |                                              |                                              |                                                        |                                                          |
| Ce γ, fcc                                                           | c              | 0                                            | 0                                            | 72.0                                                   | 26.9                                                     |
| Ce <sup>3+</sup> std. state                                         | aq             | -696.2                                       | -672.0                                       | -205.0                                                 |                                                          |
| Ce <sup>4+</sup> std. state                                         | aq             | -537.2                                       | -503.8                                       | -301.0                                                 |                                                          |
| CeCl <sub>3</sub>                                                   | c              | -1060.5                                      | -984.8                                       | 151.0                                                  | 87.4                                                     |
| std. state                                                          | aq             | -1197.5                                      | -1065.7                                      | -38.0                                                  |                                                          |
| CeF <sub>3</sub>                                                    | c              | -1635.9                                      | -1556                                        | 115.1                                                  | 99.3                                                     |
| CeI <sub>3</sub>                                                    | c              | -669.3                                       | -674                                         | 209                                                    |                                                          |
| Ce(NO <sub>3</sub> ) <sub>3</sub>                                   | c              | -1225.9                                      |                                              |                                                        |                                                          |
| CeO <sub>2</sub>                                                    | c              | -1088.7                                      | -1024.7                                      | 62.30                                                  | 61.63                                                    |
| Ce <sub>2</sub> O <sub>3</sub>                                      | c              | -1796.2                                      | -1706.2                                      | 150.6                                                  | 114.6                                                    |
| CeS                                                                 | c              | -459.4                                       | -451.5                                       | 78.2                                                   | 50.0                                                     |
| Ce <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>                     | c              | -3954.3                                      |                                              |                                                        |                                                          |
| std. state                                                          | aq             | -4176.9                                      | -3652.6                                      | -318                                                   |                                                          |
| Ce <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> · 8H <sub>2</sub> O | c              | -5522.9                                      | -5607.4                                      |                                                        |                                                          |
| Cesium                                                              |                |                                              |                                              |                                                        |                                                          |
| Cs                                                                  | c              | 0                                            | 0                                            | 85.23(40)                                              | 32.20                                                    |
|                                                                     | lq             | 2.087                                        | 0.025                                        | 92.1                                                   | 32.4                                                     |
|                                                                     | g              | 76.5(10)                                     |                                              | 175.601(3)                                             |                                                          |
| Cs <sup>+</sup> std. state                                          | aq             | -258.00(50)                                  | -292.0                                       | 132.1(5)                                               | -10.5                                                    |
| Cs acetate                                                          | aq             | -744.3                                       | -661.3                                       | 219.7                                                  |                                                          |
| CsBO <sub>2</sub>                                                   | c              | -972.0                                       | -915.0                                       | 104.4                                                  | 80.6                                                     |
| CsBr                                                                | c              | -405.8                                       | -391.4                                       | 113.05                                                 | 52.93                                                    |
| std. state                                                          | aq             | -379.8                                       | -396.0                                       | 215.5                                                  |                                                          |
| CsCl                                                                | c              | -442.8                                       | 414.4                                        | 101.18                                                 | 52.44                                                    |
| std. state                                                          | aq             | -425.4                                       | -423.3                                       | 189.4                                                  | -146.9                                                   |
| CsClO <sub>4</sub>                                                  | c              | -443.1                                       | -314.3                                       | 175.1                                                  | 108.3                                                    |
| Cs <sub>2</sub> CO <sub>3</sub>                                     | c              | -1139.7                                      | -1054.4                                      | 204.5                                                  | 123.9                                                    |
| std. state                                                          | aq             | -1193.7                                      | -1111.9                                      | 209.2                                                  |                                                          |
| CsF                                                                 | c              | -553.5                                       | -525.5                                       | 92.8                                                   | 51.1                                                     |
| std. state                                                          | aq             | -590.9                                       | -570.8                                       | 119.2                                                  |                                                          |
| Cs formate                                                          | aq             | -683.8                                       | -643.0                                       | 226.0                                                  |                                                          |
| CsHCO <sub>3</sub>                                                  | c              | -966.1                                       |                                              |                                                        |                                                          |
| CsHF                                                                | c              | -923.8                                       | -858.9                                       | 135.2                                                  | 87.3                                                     |
| CsHSO <sub>4</sub>                                                  | c              | -1158.1                                      |                                              |                                                        |                                                          |
|                                                                     | aq             | -1145.6                                      | -1047.9                                      | 264.8                                                  |                                                          |
| CsI                                                                 | c              | -346.6                                       | -340.6                                       | 123.1                                                  | 52.8                                                     |
| std. state                                                          | aq             | -313.5                                       | -343.6                                       | 244.4                                                  | -152.7                                                   |
| CsIO <sub>3</sub>                                                   | c              | -525.9                                       | -433.9                                       |                                                        | 167                                                      |
| CsNO <sub>3</sub>                                                   | c              | -506.0                                       | -406.6                                       | 155.2                                                  |                                                          |
| std. state                                                          | aq             | -465.6                                       | -403.3                                       | 279.5                                                  | -99.2                                                    |
| Cs <sub>2</sub> O                                                   | c              | -345.8                                       | -308.2                                       | 146.9                                                  | 76.0                                                     |
| CsOH                                                                | c              | -417.2                                       | 370.7                                        | 98.7                                                   | 67.9                                                     |
| std. state                                                          | aq             | -488.3                                       | -449.3                                       | 122.3                                                  |                                                          |
| Cs <sub>2</sub> PtCl <sub>6</sub> std. state                        | aq             | -1184.9                                      | -1066.9                                      | 485.8                                                  |                                                          |
| Cs <sub>2</sub> S                                                   | aq             | -483.7                                       | -498.3                                       | 251.0                                                  |                                                          |
| Cs <sub>2</sub> Se                                                  | aq             |                                              | 454.8                                        |                                                        |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                               | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|---------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Cs <sub>2</sub> SO <sub>4</sub>                         | c              | -1443.0                                      | -1323.6                                      | 211.9                                                  | 134.9                                                    |
| std. state                                              | aq             | -1425.8                                      | -1328.6                                      | 286.2                                                  |                                                          |
| Chlorine                                                |                |                                              |                                              |                                                        |                                                          |
| Cl atomic                                               | g              | 121.301(8)                                   |                                              | 165.190(4)                                             |                                                          |
| Cl <sup>-</sup> std. state                              | aq             | -167.08(10)                                  | -131.3                                       | 56.60(20)                                              | -136.4                                                   |
| Cl <sub>2</sub>                                         | g              | 0                                            | 0                                            | 233.08(10)                                             | 33.95                                                    |
| ClF                                                     | g              | -50.3                                        | -51.84                                       | 217.9                                                  | 32.08                                                    |
| ClF <sub>3</sub>                                        | g              | -163.2                                       | -123.0                                       | 281.6                                                  | 63.85                                                    |
| ClF <sub>5</sub>                                        | g              | -239                                         | -147                                         | 310.74                                                 | 97.17                                                    |
| ClO                                                     | g              | 101.8                                        | 98.1                                         | 226.6                                                  | 31.5                                                     |
| ClO <sup>-</sup> std. state                             | aq             | -107.1                                       | -36.8                                        | 41.8                                                   |                                                          |
| ClO <sub>2</sub>                                        | g              | 102.5                                        | 120.5                                        | 256.8                                                  | 42.00                                                    |
| ClO <sub>2</sub> <sup>-</sup> std. state                | aq             | -66.5                                        | 17.2                                         | 101.3                                                  |                                                          |
| ClO <sub>3</sub> <sup>-</sup> std. state                | aq             | -104.0                                       | -8.0                                         | 162.3                                                  |                                                          |
| ClO <sub>3</sub> F perchloryl fluoride                  | g              | -23.8                                        | 48.2                                         | 279.0                                                  | 64.9                                                     |
| ClO <sub>4</sub> <sup>-</sup> std. state                | aq             | -128.10(40)                                  | -8.62                                        | 184.0(15)                                              |                                                          |
| Cl <sub>2</sub> O                                       | g              | 80.3                                         | 97.9                                         | 266.2                                                  | 45.4                                                     |
| Cl <sub>2</sub> O <sub>7</sub>                          | lq             | 238.1                                        |                                              |                                                        |                                                          |
|                                                         | g              | 1138                                         |                                              |                                                        |                                                          |
| Chromium                                                |                |                                              |                                              |                                                        |                                                          |
| Cr                                                      | c              | 0                                            | 0                                            | 23.8                                                   | 23.43                                                    |
| Cr <sup>2+</sup> std. state                             | aq             | -143.5                                       |                                              |                                                        |                                                          |
| CrBr <sub>2</sub>                                       | c              | -302.1                                       |                                              |                                                        |                                                          |
| CrCl <sub>2</sub>                                       | c              | -395.4                                       | -356.0                                       | 115.3                                                  | 71.2                                                     |
| CrCl <sub>3</sub>                                       | c              | -556.5                                       | -486.1                                       | 123.0                                                  | 91.8                                                     |
| Cr(CO) <sub>6</sub> hexacarbonyl                        | c              | -1077.8                                      |                                              | 293.01                                                 | 226.23                                                   |
| CrF <sub>2</sub>                                        | c              | -778.0                                       |                                              |                                                        |                                                          |
| CrF <sub>3</sub>                                        | c              | -1159                                        | -1088                                        | 93.9                                                   | 78.7                                                     |
| Cr <sub>2</sub> FeO <sub>4</sub>                        | c              | -1444.7                                      | -1343.8                                      | 146.0                                                  | 133.6                                                    |
| CrI <sub>2</sub>                                        | c              | -156.9                                       |                                              |                                                        |                                                          |
| CrI <sub>3</sub>                                        | c              | -205.0                                       |                                              |                                                        |                                                          |
| CrN                                                     | c              | -117                                         | -93                                          | 38                                                     | 52.7                                                     |
| CrO <sub>2</sub>                                        | c              | -598.0                                       |                                              |                                                        |                                                          |
| Cr <sub>2</sub> O <sub>3</sub>                          | c              | -1140                                        | -1058.1                                      | 81.2                                                   | 118.7                                                    |
| Cr <sub>3</sub> O <sub>4</sub>                          | c              | -1131.0                                      |                                              |                                                        |                                                          |
| CrO <sub>2</sub> Cl <sub>2</sub>                        | g              | -538.1                                       | -501.6                                       | 329.8                                                  | 84.5                                                     |
| CrO <sub>4</sub> <sup>2-</sup> std. state               | aq             | -881.15                                      | -727.85                                      | 50.21                                                  |                                                          |
| HCrO <sub>4</sub> <sup>-</sup> std. state               | aq             | -878.22                                      | -764.84                                      | 184.1                                                  |                                                          |
| Cr <sub>2</sub> O <sub>7</sub> <sup>2-</sup> std. state | aq             | -1490.3                                      | -1301.2                                      | 261.9                                                  |                                                          |
| Cr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>         | c              | -609.6                                       |                                              | 269.9                                                  | 302.6                                                    |
| Cobalt                                                  |                |                                              |                                              |                                                        |                                                          |
| Co                                                      | c              | 0                                            | 0                                            | 30.0                                                   | 24.8                                                     |
| Co <sup>2+</sup> std. state                             | aq             | -58.2                                        | -54.4                                        | -113                                                   |                                                          |
| Co <sup>3+</sup> std. state                             | aq             | 92                                           | 134                                          | -305                                                   |                                                          |
| CoBr <sub>2</sub>                                       | c              | -220.9                                       |                                              |                                                        | 79.5                                                     |
| std. state                                              | aq             | -301.3                                       | -262.3                                       | 50                                                     |                                                          |
| CoCl <sub>2</sub>                                       | c              | -312.5                                       | -269.8                                       | 109.2                                                  | 78.49                                                    |
| std. state                                              | aq             | -392.5                                       | -316.7                                       | 0                                                      |                                                          |
| CoCO <sub>3</sub>                                       | c              | -713.0                                       |                                              |                                                        |                                                          |
| CoF <sub>2</sub>                                        | c              | -692                                         | -647                                         | 82.4                                                   | 68.9                                                     |
| CoF <sub>3</sub>                                        | c              | -790                                         | -719                                         | 95                                                     | 92                                                       |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                   | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| CoI <sub>2</sub>                                            | c              | -88.7                                        |                                              |                                                        |                                                          |
|                                                             | aq             | -168.6                                       | -157.7                                       | 109.0                                                  |                                                          |
| Co(NH <sub>3</sub> ) <sub>6</sub> <sup>2+</sup> std. state  | aq             | -584.9                                       | -157.3                                       | 146                                                    |                                                          |
| Co(NH <sub>3</sub> ) <sub>6</sub> <sup>3+</sup> std. state  | aq             |                                              | -189.5                                       |                                                        |                                                          |
| Co(NO <sub>3</sub> ) <sub>2</sub>                           | c              | -420.5                                       |                                              |                                                        |                                                          |
| std. state                                                  | aq             | -472.8                                       | -277.0                                       | 180                                                    |                                                          |
| CoO                                                         | c              | -237.7                                       | -214.0                                       | 53.0                                                   | 55.3                                                     |
| Co <sub>3</sub> O <sub>4</sub>                              | c              | -891                                         | -774                                         | 102.5                                                  | 123.4                                                    |
| Co(OH) <sub>2</sub>                                         | c              | -539.7                                       | -454.4                                       | 79.0                                                   |                                                          |
| CoS                                                         | c              | -82.8                                        |                                              |                                                        |                                                          |
| Co <sub>2</sub> S <sub>3</sub>                              | c              | -147.3                                       |                                              |                                                        |                                                          |
| CoSO <sub>4</sub>                                           | c              | -888.3                                       | -782.4                                       | 118.0                                                  | 103                                                      |
| std. state                                                  | aq             | -967.3                                       | -799.1                                       | -92.0                                                  |                                                          |
| CoSO <sub>4</sub> · 7H <sub>2</sub> O                       | c              | -2979.93                                     | -2473.83                                     | 406.06                                                 | 390.49                                                   |
| Copper                                                      |                |                                              |                                              |                                                        |                                                          |
| Cu                                                          | c              | 0                                            | 0                                            | 33.15(8)                                               | 24.44                                                    |
|                                                             | g              | 337.4(12)                                    |                                              | 166.398(4)                                             |                                                          |
| Cu <sup>+</sup> std. state                                  | aq             | 71.67                                        | 50.00                                        | 40.6                                                   |                                                          |
| Cu <sup>2+</sup> std. state                                 | aq             | 64.9(10)                                     | 65.52                                        | -98.(4)                                                |                                                          |
| Cu(OAc) <sub>2</sub> acetate                                | c              | -893.3                                       |                                              |                                                        |                                                          |
| std. state                                                  | aq             | -907.25                                      | -673.29                                      | 73.6                                                   |                                                          |
| Cu <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> std. state | aq             | -1581.97                                     | -1100.48                                     | -804.2                                                 |                                                          |
| CuBr                                                        | c              | -104.6                                       | -100.8                                       | 96.2                                                   | 54.7                                                     |
| CuBr <sub>2</sub>                                           | c              | -141.84                                      |                                              |                                                        |                                                          |
| CuCl                                                        | c              | -137.2                                       | -119.9                                       | 86.2                                                   | 48.5                                                     |
| CuCl <sub>2</sub>                                           | c              | -220.1                                       | -175.7                                       | 108.09                                                 | 71.88                                                    |
| Cu(ClO <sub>4</sub> ) <sub>2</sub> std. state               | aq             | -193.89                                      | 48.28                                        | 264.4                                                  |                                                          |
| CuCN                                                        | c              | 95.0                                         | 108.4                                        | 90.00                                                  | 61.04                                                    |
| CuCNS std. state                                            | aq             | 138.11                                       | 142.67                                       | 184.93                                                 |                                                          |
| Cu(CNS) <sub>2</sub> std. state                             | aq             | 217.65                                       | 250.87                                       | 189.1                                                  |                                                          |
| CuF                                                         | c              | -280                                         | -260                                         | 64.9                                                   | 51.9                                                     |
| CuF <sub>2</sub>                                            | c              | -542.7                                       | -492                                         | 77.45                                                  | 65.55                                                    |
| Cu(formate) <sub>2</sub>                                    | aq             | -786.34                                      | -636.4                                       | 84                                                     |                                                          |
| CuI                                                         | c              | 67.8                                         | -69.5                                        | 96.7                                                   | 54.1                                                     |
| Cu(NH <sub>3</sub> ) <sub>4</sub> <sup>2+</sup> std. state  | aq             | -348.5                                       | -111.3                                       | 273.6                                                  |                                                          |
| Cu(NO <sub>3</sub> ) <sub>2</sub>                           | c              | -302.9                                       |                                              |                                                        |                                                          |
| std. state                                                  | aq             | -349.95                                      | -157.15                                      | 193.3                                                  |                                                          |
| CuO                                                         | c              | -157.3                                       | -129.7                                       | 42.6                                                   | 42.2                                                     |
| Cu <sub>2</sub> O                                           | c              | -168.6                                       | -149.0                                       | 93.1                                                   | 63.6                                                     |
| Cu(OH) <sub>2</sub>                                         | c              | -450                                         | -373                                         | 108.4                                                  | 95.19                                                    |
| CuS                                                         | c              | -53.1                                        | -53.7                                        | 66.5                                                   | 47.8                                                     |
| Cu <sub>2</sub> S                                           | c              | -79.5                                        | -86.2                                        | 120.9                                                  | 76.3                                                     |
| CuSe                                                        | c              | -39.5                                        |                                              |                                                        |                                                          |
| Cu <sub>2</sub> Se                                          | c              | -59.4                                        |                                              | 157.3                                                  | 88.70                                                    |
| CuSO <sub>4</sub>                                           | c              | -771.4(12)                                   | -662.2                                       | 109.2(4)                                               | 98.87                                                    |
| std. state                                                  | aq             | -844.50                                      | -679.11                                      | -79.5                                                  |                                                          |
| CuSO <sub>4</sub> · 5H <sub>2</sub> O                       | c              | -2279.65                                     | -1880.04                                     | 300.4                                                  | 280                                                      |
| CuWO <sub>4</sub>                                           | c              | -1105.0                                      |                                              |                                                        |                                                          |
| Dysprosium                                                  |                |                                              |                                              |                                                        |                                                          |
| Dy                                                          | c              | 0                                            | 0                                            | 75.6                                                   | 27.7                                                     |
| Dy <sup>3+</sup> std. state                                 | aq             | -699.0                                       | -665.0                                       | -231.0                                                 | 21.0                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                 | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| DyCl <sub>3</sub>                         | c              | −1000                                        |                                              |                                                        | 100.0                                                    |
|                                           | aq             | −1197.0                                      | −1059.0                                      | −61.9                                                  | −389.0                                                   |
| DyF <sub>3</sub>                          | c              | −1711.0                                      |                                              |                                                        |                                                          |
| Dy <sub>2</sub> O <sub>3</sub>            | c              | −1863.1                                      | −1771.5                                      | 149.8                                                  | 116.27                                                   |
| Erbium                                    |                |                                              |                                              |                                                        |                                                          |
| Er                                        | c              | 0                                            | 0                                            | 73.18                                                  | 28.12                                                    |
| Er <sup>3+</sup> std. state               | aq             | −705.4                                       | −669.1                                       | −244.3                                                 | 21.0                                                     |
| ErCl <sub>3</sub>                         | c              | −998.7                                       |                                              |                                                        | 100.0                                                    |
|                                           | aq             | −1207.1                                      | −1062.7                                      | −75.3                                                  | −389.0                                                   |
| Er <sub>2</sub> O <sub>3</sub>            | c              | −1897.9                                      | −1808.7                                      | 155.6                                                  | 108.49                                                   |
| Europium                                  |                |                                              |                                              |                                                        |                                                          |
| Eu                                        | c              | 0                                            | 0                                            | 77.78                                                  | 27.66                                                    |
| Eu <sup>2+</sup> std. state               | aq             | −527.0                                       | 540.2                                        | −8.0                                                   |                                                          |
| Eu <sup>3+</sup>                          | aq             | −605.0                                       | −574.0                                       | −222.0                                                 | 8.0                                                      |
| EuCl <sub>2</sub>                         | aq             | −862.0                                       |                                              |                                                        |                                                          |
| EuCl <sub>3</sub>                         | c              | −936.0                                       | −856                                         | 144.1                                                  |                                                          |
|                                           | aq             | −1106.2                                      | −967.7                                       | −54.0                                                  | −402.0                                                   |
| EuF <sub>3</sub>                          | c              | −1571                                        |                                              |                                                        |                                                          |
| Eu <sub>2</sub> O <sub>3</sub> monoclinic | c              | −1651.4                                      | −1556.9                                      | 146                                                    | 122.2                                                    |
| Eu <sub>3</sub> O <sub>4</sub>            | c              | −2272.0                                      | −2142.0                                      | 205.0                                                  |                                                          |
| Eu(OH) <sub>3</sub>                       | c              | −1332                                        | −1195                                        | 119.9                                                  |                                                          |
| Fluorine                                  |                |                                              |                                              |                                                        |                                                          |
| F atomic                                  | g              | 79.38(30)                                    | 62.3                                         | 158.751(4)                                             | 22.7                                                     |
| F <sup>−</sup>                            | aq             | −335.35(65)                                  | −278.8                                       | −13.8(8)                                               | −106.7                                                   |
| F <sub>2</sub>                            | g              | 0                                            | 0                                            | 202.791(5)                                             | 31.30                                                    |
| FNO <sub>3</sub>                          | g              | 10.5                                         | 73.7                                         | 292.9                                                  | 65.22                                                    |
| FO                                        | g              | 109.0                                        | 105.0                                        | 216.8                                                  | 30.5                                                     |
| F <sub>2</sub> O                          | g              | 24.7                                         | 41.9                                         | 247.4                                                  | 43.3                                                     |
| F <sub>2</sub> O <sub>2</sub>             | g              | 18.0                                         |                                              |                                                        |                                                          |
| Francium                                  |                |                                              |                                              |                                                        |                                                          |
| Fr                                        | c              | 0                                            | 0                                            | 95.40                                                  | 31.80                                                    |
| FrCl                                      | c              | −439                                         |                                              | 113.0                                                  | 53.56                                                    |
| Fr <sub>2</sub> O                         | c              | −338                                         | 299.2                                        | 156.9                                                  |                                                          |
| Gadolinium                                |                |                                              |                                              |                                                        |                                                          |
| Gd                                        | c              | 0                                            | 0                                            | 68.07                                                  | 37.03                                                    |
| Gd <sup>3+</sup> std. state               | aq             | −686.0                                       | −661.0                                       | −205.9                                                 |                                                          |
| GdCl <sub>3</sub>                         | c              | −1008.0                                      | −933                                         | 151.4                                                  | 88.0                                                     |
| std. state                                | aq             | −1188.0                                      | −1059.0                                      | −36.8                                                  | −410.0                                                   |
| GdF <sub>3</sub>                          | lq             | −1297                                        |                                              |                                                        |                                                          |
| Gd <sub>2</sub> O <sub>3</sub> monoclinic | c              | −1819.6                                      | −1730                                        | 150.6                                                  | 106.7                                                    |
| Gallium                                   |                |                                              |                                              |                                                        |                                                          |
| Ga                                        | c              | 0                                            | 0                                            | 40.8                                                   | 26.06                                                    |
|                                           | lq             | 5.6                                          |                                              |                                                        |                                                          |
|                                           | g              | 272.0                                        | 233.7                                        | 169.0                                                  | 25.3                                                     |
| Ga <sup>3+</sup>                          | aq             | −211.7                                       | −159.0                                       | −331.0                                                 |                                                          |
| GaAs                                      | c              | −71.0                                        | −67.8                                        | 64.2                                                   | 46.2                                                     |
| GaBr <sub>3</sub>                         | c              | −386.6                                       | −359.8                                       | 180.0                                                  |                                                          |
| GaCl <sub>3</sub>                         | c              | −524.7                                       | −454.8                                       | 142.0                                                  |                                                          |
| GaF <sub>3</sub>                          | c              | −1163.0                                      | −1085.3                                      | 84                                                     |                                                          |
| GaI <sub>3</sub>                          | c              | −238.9                                       |                                              | 205.0                                                  | 100                                                      |
| Ga <sub>2</sub> O <sub>3</sub> rhombic    | c              | −1089.1                                      | −998.3                                       | 84.98                                                  | 92.1                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                               | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|---------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Ga(OH) <sub>3</sub>                                     | c              | -964.4                                       | -831.3                                       | 100.0                                                  |                                                          |
| GaSb                                                    | c              | -41.8                                        | -38.9                                        | 76.07                                                  | 48.53                                                    |
| Germanium                                               |                |                                              |                                              |                                                        |                                                          |
| Ge                                                      | c              | 0                                            | 0                                            | 31.09(15)                                              | 23.3                                                     |
|                                                         | g              | 372.0(30)                                    | 331.2                                        | 167.904(5)                                             | 30.7                                                     |
| GeBr <sub>4</sub>                                       | lq             | -347.7                                       | -331.4                                       | 280.8                                                  |                                                          |
|                                                         | g              | -300.0                                       | -318.0                                       | 396.2                                                  | 101.8                                                    |
| GeCl <sub>4</sub>                                       | lq             | -531.8                                       | -462.8                                       | 245.6                                                  |                                                          |
|                                                         | g              | -495.8                                       | -457.3                                       | 347.7                                                  | 96.1                                                     |
| GeF <sub>4</sub>                                        | g              | -1190.20(50)                                 | -1150.0                                      | 301.9(10)                                              | 81.84                                                    |
| GeH <sub>4</sub>                                        | g              | 90.8                                         | 113.4                                        | 217.02                                                 | 45.02                                                    |
| GeI <sub>4</sub>                                        | c              | -141.8                                       | -144.4                                       | 271.1                                                  |                                                          |
|                                                         | g              | -56.9                                        | -106.3                                       | 428.9                                                  | 104.1                                                    |
| GeO <sub>2</sub> tetragonal                             | c              | -580.0(10)                                   | -521.4                                       | 39.71(15)                                              | 52.1                                                     |
| GeP                                                     | c              | -21.0                                        | -17.0                                        | 63.0                                                   |                                                          |
| GeS                                                     | c              | -69.0                                        | -71.6                                        | 71                                                     |                                                          |
| Gold                                                    |                |                                              |                                              |                                                        |                                                          |
| Au                                                      | c              | 0                                            | 0                                            | 47.4                                                   | 25.36                                                    |
| AuBr                                                    | c              | -14.0                                        |                                              |                                                        |                                                          |
| AuBr <sub>3</sub>                                       | c              | -53.3                                        |                                              |                                                        |                                                          |
| AuCl                                                    | c              | -34.7                                        |                                              | 92.9                                                   | 48.74                                                    |
| AuCl <sub>3</sub>                                       | c              | -117.6                                       |                                              | 148.1                                                  | 94.81                                                    |
| AuCl <sub>4</sub> std. state                            | aq             | -322.2                                       | -237.32                                      | 266.9                                                  |                                                          |
| Au(CN) <sub>2</sub> std. state                          | aq             | 242.3                                        | 285.8                                        | 172                                                    |                                                          |
| AuF <sub>3</sub>                                        | c              | -363.6                                       |                                              | 114.2                                                  | 91.29                                                    |
| AuSb <sub>2</sub>                                       | c              | -19.46                                       |                                              | 119.2                                                  | 77.40                                                    |
| AuSn                                                    | c              | -30.5                                        |                                              | 93.7                                                   | 49.41                                                    |
| Hafnium                                                 |                |                                              |                                              |                                                        |                                                          |
| Hf hexagonal                                            | c              | 0                                            | 0                                            | 43.56                                                  | 25.69                                                    |
| HfC                                                     | c              | -230.1                                       |                                              | 41.21                                                  | 34.43                                                    |
| HfCl <sub>4</sub>                                       | c              | -990.4                                       | -901.3                                       | 190.8                                                  | 120.46                                                   |
| HfF <sub>4</sub> monoclinic                             | c              | -1930.5                                      | -1830.5                                      | 113                                                    |                                                          |
| HfO <sub>2</sub>                                        | c              | -1144.7                                      | -1088.2                                      | 59.3                                                   | 60.25                                                    |
| Helium                                                  |                |                                              |                                              |                                                        |                                                          |
| He                                                      | g              | 0                                            | 0                                            | 126.153(2)                                             | 20.786                                                   |
| Holmium                                                 |                |                                              |                                              |                                                        |                                                          |
| Ho                                                      | c              | 0                                            | 0                                            | 75.3                                                   | 27.15                                                    |
| Ho <sup>3+</sup> std. state                             | aq             | -705.0                                       | -673.7                                       | 226.8                                                  | 17.0                                                     |
| HoCl <sub>3</sub>                                       | c              | -1005.4                                      |                                              |                                                        | 88                                                       |
| std. state                                              | aq             | -1206.7                                      | -1067.3                                      | -57.7                                                  | -393.0                                                   |
| HoF <sub>3</sub>                                        | c              | -1707.0                                      |                                              |                                                        |                                                          |
| Ho <sub>2</sub> O <sub>3</sub>                          | c              | -1880.7                                      | -1791.2                                      | 158.2                                                  | 115.0                                                    |
| Hydrogen                                                |                |                                              |                                              |                                                        |                                                          |
| H atomic                                                | g              | 217.998(6)                                   | 203.3                                        | 114.717(2)                                             | 20.8                                                     |
| H <sup>+</sup> std. state                               | aq             | 0                                            | 0                                            | 0                                                      | 0                                                        |
| H <sub>2</sub>                                          | g              | 0                                            | 0                                            | 130.680(3)                                             | 28.84                                                    |
| H <sup>2</sup> H                                        | g              | 0.321                                        | -1.463                                       | 143.80                                                 | 29.20                                                    |
| <sup>2</sup> H <sub>2</sub> (D <sub>2</sub> ) deuterium | g              | 0                                            | 0                                            | 144.96                                                 | 29.19                                                    |
| HAsO <sub>2</sub> undissoc;<br>std. state               | aq             | -456.5                                       | -402.71                                      | 125.9                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                         | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| H <sub>2</sub> AsO <sub>3</sub> <sup>-</sup> undissoc; std. state | aq             | -714.79                                      | -587.22                                      | 110.5                                                  |                                                          |
| H <sub>3</sub> AsO <sub>3</sub> undissoc; std. state              | aq             | -742.2                                       | -639.90                                      | 195.0                                                  |                                                          |
| HAAsO <sub>4</sub> <sup>2-</sup> undissoc; std. state             | aq             | -906.34                                      | -714.70                                      | -1.7                                                   |                                                          |
| H <sub>2</sub> AsO <sub>4</sub> <sup>-</sup> undissoc; std. state | aq             | -909.56                                      | -753.29                                      | 117                                                    |                                                          |
| H <sub>3</sub> AsO <sub>3</sub>                                   | c              | -906.30                                      |                                              |                                                        |                                                          |
| undissoc; std. state                                              | aq             | -902.5                                       | -766.1                                       | 184                                                    |                                                          |
| HBO <sub>2</sub>                                                  | c              | -794.3                                       | -723.4                                       | 38                                                     | 54.4                                                     |
| H <sub>3</sub> BO <sub>3</sub>                                    | c              | -1094.8(8)                                   | -968.9                                       | 89.95(60)                                              | 86.1                                                     |
| undissoc                                                          | aq             | -1072.8(8)                                   |                                              | 162.4(6)                                               |                                                          |
| HBr                                                               | g              | -36.29(16)                                   | -53.4                                        | 198.700(4)                                             | 29.1                                                     |
| std. state                                                        | aq             | -121.55                                      | -103.97                                      | 82.4                                                   | -141.8                                                   |
| HBrO undissoc; std. state                                         | aq             | -113.0                                       | -82.4                                        | 142                                                    |                                                          |
| HBrO <sub>3</sub> std. state                                      | aq             | -67.07                                       | 18.54                                        | 161.71                                                 |                                                          |
| HCl                                                               | g              | -92.31(10)                                   | -95.30                                       | 186.902(5)                                             | 29.12                                                    |
| std. state                                                        | aq             | -167.15                                      | -131.25                                      | 56.5                                                   | -136.4                                                   |
| <sup>2</sup> HCl deuterium chloride                               | g              | -93.35                                       | -95.94                                       | 192.63                                                 | 29.17                                                    |
| HCIO                                                              | g              | -78.7                                        | -66.1                                        | 236.7                                                  | 37.15                                                    |
| undissoc; std. state                                              | aq             | -120.9                                       | -79.9                                        | 142                                                    |                                                          |
| HCIO <sub>2</sub> undissoc; std. state                            | aq             | -51.9                                        | 5.9                                          | 188.3                                                  |                                                          |
| HCIO <sub>3</sub> std. state                                      | aq             | -103.97                                      | -8.03                                        | 162.3                                                  |                                                          |
| HCIO <sub>4</sub>                                                 | lq             | -40.58                                       |                                              |                                                        |                                                          |
| std. state                                                        | aq             | -129.33                                      | -8.62                                        | 182.0                                                  |                                                          |
| HCIO <sub>4</sub> · H <sub>2</sub> O                              | c              | -302.21                                      |                                              |                                                        |                                                          |
| HCIO <sub>4</sub> · 2H <sub>2</sub> O                             | lq             | -677.98                                      |                                              |                                                        |                                                          |
| HCN                                                               | lq             | 108.87                                       | 124.93                                       | 112.84                                                 | 70.63                                                    |
|                                                                   | g              | 135.1                                        | 124.7                                        | 201.81                                                 | 35.86                                                    |
| ionized; std. state                                               | aq             | 150.6                                        | 172.4                                        | 94.1                                                   |                                                          |
| undissoc; std. state                                              | aq             | 107.11                                       | 119.66                                       | 124.7                                                  |                                                          |
| HCNO ionized; std. state                                          | aq             | -146.0                                       | -97.5                                        | 106.7                                                  |                                                          |
| undissoc; std. state                                              | aq             | -154.39                                      | -117.2                                       | 144.8                                                  |                                                          |
| HCNS ionized; std. state                                          | aq             | 76.44                                        | 92.68                                        | 144.4                                                  | -40.2                                                    |
| HCOO <sup>-</sup> formate                                         | aq             | -425.6                                       | -351.0                                       | 92.0                                                   | -87.9                                                    |
| CH <sub>3</sub> COO <sup>-</sup> acetate                          | aq             | -486.0                                       | -369.3                                       | 86.6                                                   | -6.3                                                     |
| HCO <sub>3</sub> <sup>-</sup> std. state                          | aq             | -689.93(20)                                  | -586.85                                      | 98.4(5)                                                |                                                          |
| H <sub>2</sub> CO <sub>3</sub> std. state                         | aq             | -699.65                                      | -623.16                                      | 187.4                                                  |                                                          |
| HC <sub>2</sub> O <sub>4</sub> <sup>-</sup>                       | aq             | -818.4                                       | -698.3                                       | 149.4                                                  |                                                          |
| H <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                      | c              | -821.7                                       | -723.7                                       | 109.8                                                  | 91.0                                                     |
| C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>                       | aq             | -825.1                                       | -673.9                                       | 45.6                                                   |                                                          |
| H <sub>2</sub> C <sub>3</sub> S <sub>3</sub> trithiocarbonic acid | lq             | 25.1                                         | 27.82                                        | 233.0                                                  | 149.8                                                    |
| HF                                                                | g              | -273.30(70)                                  | -275.4                                       | 173.779(3)                                             | 29.14                                                    |
|                                                                   | lq             | -299.78                                      | 75.40                                        | 51.67                                                  |                                                          |
| undissoc; std. state                                              | aq             | -320.08                                      | -296.86                                      | 88.7                                                   |                                                          |
| F <sup>-</sup>                                                    | aq             | -332.63                                      | -278.8                                       | -13.8                                                  | -106.7                                                   |
| <sup>2</sup> HF                                                   | g              | -275.5                                       | -277.27                                      | 179.70                                                 | 29.14                                                    |
| HF <sub>2</sub> std. state                                        | aq             | -649.94                                      | -578.15                                      | 92.5                                                   |                                                          |
| H <sub>2</sub> F <sub>2</sub> dimer                               | g              | -572.66                                      | -544.51                                      | 238                                                    | 44.89                                                    |
| H <sub>2</sub> Fe(CN) <sub>6</sub> <sup>-</sup> std. state        | aq             | 455.6                                        | 658.44                                       | 218                                                    |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                      | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| HFO                                                            | g              | 98                                           | -86                                          | 226.8                                                  | 35.93                                                    |
| HI                                                             | g              | 26.50(10)                                    | 1.7                                          | 206.590(4)                                             | 29.16                                                    |
| std. state                                                     | aq             | -55.19                                       | -51.59                                       | 111.3                                                  | -142.3                                                   |
| HIO undissoc; std. state                                       | aq             | -138.1                                       | -99.2                                        | 95.4                                                   |                                                          |
| HIO <sub>3</sub>                                               | c              | -230.1                                       |                                              |                                                        |                                                          |
| H <sub>2</sub> MoO <sub>4</sub>                                | c              | -1046.0                                      |                                              |                                                        |                                                          |
| HN                                                             | g              | 351.5                                        | 345.6                                        | 181.2                                                  | 29.2                                                     |
| HN <sub>3</sub>                                                | lq             | 264.0                                        | 327.2                                        | 140.6                                                  |                                                          |
|                                                                | g              | 294.1                                        | 328.1                                        | 239.0                                                  | 43.7                                                     |
| H <sub>2</sub> N                                               | g              | 184.9                                        | 194.6                                        | 195.0                                                  | 33.9                                                     |
| <sup>2</sup> H <sub>2</sub> N <sub>2</sub> <i>cis</i> -diazine | g              | 207                                          | 241                                          | 224.09                                                 | 39.02                                                    |
| HNCO isocyanic acid                                            | g              | -116.73                                      | -107.36                                      | 238.11                                                 | 44.85                                                    |
| HNCS isothiocyanic acid                                        | g              | 127.61                                       | 112.88                                       | 248.03                                                 | 46.40                                                    |
| HNO <sub>2</sub>                                               | g              | -79.5                                        | -46.0                                        | 254.1                                                  | 45.5                                                     |
| HNO <sub>3</sub>                                               | lq             | -174.1                                       | -80.7                                        | 155.60                                                 | 109.9                                                    |
|                                                                | g              | -133.9                                       | -73.54                                       | 266.9                                                  | 54.1                                                     |
| std. state                                                     | aq             | -207.36                                      | -111.34                                      | 146.4                                                  | -86.6                                                    |
| H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> hyponitrous acid  | aq             | -57.3                                        | 36.0                                         | 218                                                    |                                                          |
| HO hydroxyl                                                    | g              | 39.0                                         | 34.2                                         | 183.64                                                 | 30.00                                                    |
| HO <sup>-</sup>                                                | aq             | -230.015                                     | -157.28                                      | -10.90                                                 | -148.5                                                   |
| HO <sub>2</sub>                                                | g              | 10.5                                         | 22.6                                         | 229.0                                                  | 34.9                                                     |
| HO <sub>2</sub> <sup>-</sup> std. state                        | aq             | -160.33                                      | 67.4                                         | 23.9                                                   |                                                          |
| H <sub>2</sub> O                                               | c              | -292.72                                      |                                              |                                                        | 37.11                                                    |
|                                                                | lq             | -285.830(40)                                 | -237.14                                      | 69.95(3)                                               | 75.35                                                    |
|                                                                | g              | -241.826(40)                                 | -228.61                                      | 188.835(10)                                            | 33.60                                                    |
| <sup>1</sup> H <sup>2</sup> HO                                 | g              | -245.37                                      | -233.18                                      | 199.51                                                 | 33.79                                                    |
| <sup>2</sup> H <sub>2</sub> O deuterium oxide                  | g              | -249.20                                      | -234.54                                      | 198.33                                                 | 34.25                                                    |
| H <sub>2</sub> O <sub>2</sub> hydrogen peroxide                | lq             | -187.78                                      | -120.42                                      | 109.6                                                  | 89.1                                                     |
|                                                                | g              | -136.3                                       | -105.6                                       | 232.7                                                  | 43.14                                                    |
| undissoc; std. state                                           | aq             | -191.17                                      | -134.10                                      | 143.9                                                  |                                                          |
| HOCN undissoc; std. state                                      | aq             | -154.39                                      | -117.2                                       | 144.8                                                  |                                                          |
| OCN <sup>-</sup> cyanate std. state                            | aq             | -146.02                                      | -97.5                                        | 106.7                                                  |                                                          |
| HPO <sub>3</sub>                                               | c              | -948.51                                      |                                              |                                                        |                                                          |
| HPO <sub>4</sub> <sup>2-</sup> std. state                      | aq             | -1299.0(15)                                  | -1089.26                                     | -33.5(15)                                              |                                                          |
| H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> std. state         | aq             | -1302.6(15)                                  | -1130.39                                     | 92.5(15)                                               |                                                          |
| HPH <sub>2</sub> O <sub>2</sub> hypophosphorous acid           | c              | -604.6                                       |                                              |                                                        |                                                          |
| H <sub>3</sub> PO <sub>3</sub>                                 | c              | -964.4                                       |                                              |                                                        |                                                          |
| H <sub>3</sub> PO <sub>4</sub>                                 | c              | -1284.4                                      | -1124.3                                      | 110.5                                                  | 106.1                                                    |
|                                                                | lq             | -1271.7                                      | -1123.6                                      | 150.8                                                  | 145.06                                                   |
| ionized; std. state                                            | aq             | -1277.4                                      | -1018.8                                      | 222                                                    |                                                          |
| undissoc; std. state                                           | aq             | -1288.34                                     | -1142.65                                     | 158.2                                                  |                                                          |
| HP <sub>2</sub> O <sub>3</sub> <sup>3-</sup>                   | aq             | -2274.8                                      | -1972.2                                      | 46.0                                                   |                                                          |
| H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> <sup>4-</sup>     | aq             | -2278.6                                      | -2010.2                                      | 163.0                                                  |                                                          |
| H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>                   | c              | -2241.0                                      |                                              |                                                        |                                                          |
| undissoc; std. state                                           | aq             | -2268.6                                      | -2032.2                                      | 268                                                    |                                                          |
| HReO <sub>4</sub>                                              | c              | -762.3                                       | -656.4                                       | 158.2                                                  |                                                          |
| HS                                                             | g              | 142.7                                        | 113.3                                        | 195.7                                                  | 32.3                                                     |
| HS <sup>-</sup> std. state                                     | aq             | -16.3(15)                                    | 12.05                                        | 67.(5)                                                 |                                                          |
| H <sub>2</sub> S                                               | g              | -20.6(5)                                     | -33.4                                        | 205.81(5)                                              | 34.19                                                    |
| undissoc; std. state                                           | aq             | -38.6(15)                                    | -27.87                                       | 126.(5)                                                |                                                          |



**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                           | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-----------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| <sup>2</sup> H <sub>2</sub> S                       | g              | - 23.9                                       | - 35.3                                       | 215.3                                                  | 35.76                                                    |
| H <sub>2</sub> S <sub>2</sub>                       | g              | 15.5                                         |                                              |                                                        | 51.5                                                     |
| HSbO <sub>2</sub> undissoc; std. state              | aq             | - 487.9                                      | - 407.5                                      | 46.6                                                   |                                                          |
| HSCN undissoc; std. state                           | aq             | 76.4                                         | 97.7                                         | 144.3                                                  | - 40.2                                                   |
| SCN <sup>-</sup> std. state                         | aq             | 76.44                                        | 92.68                                        | 144.5                                                  | - 40.2                                                   |
| HSe <sup>-</sup> std. state                         | aq             | 15.9                                         | 43.9                                         | 79.0                                                   |                                                          |
| H <sub>2</sub> Se                                   | g              | 29.7                                         | 15.9                                         | 219.0                                                  | 34.7                                                     |
| HSeO <sub>3</sub> <sup>-</sup> std. state           | aq             | - 514.55                                     | - 411.54                                     | 135.1                                                  |                                                          |
| H <sub>2</sub> SeO <sub>3</sub>                     | c              | - 524.46                                     |                                              |                                                        |                                                          |
| undissoc; std. state                                | aq             | - 507.48                                     | - 426.22                                     | 207.9                                                  |                                                          |
| HSeO <sub>4</sub> <sup>-</sup> std. state           | aq             | - 581.6                                      | - 452.3                                      | 149.4                                                  |                                                          |
| H <sub>2</sub> SeO <sub>4</sub>                     | c              | - 530.1                                      |                                              |                                                        |                                                          |
| H <sub>2</sub> SiO <sub>3</sub>                     | c              | - 1188.67                                    | - 1092.4                                     | 134.0                                                  |                                                          |
| undissoc; std. state                                | aq             | - 1182.8                                     | - 1079.5                                     | 109                                                    |                                                          |
| H <sub>4</sub> SiO <sub>4</sub>                     | c              | - 1481.1                                     | - 1333.0                                     | 192                                                    |                                                          |
| undissoc; std. state                                | aq             | - 1468.6                                     | - 1316.7                                     | 180                                                    |                                                          |
| HSO <sub>3</sub> <sup>-</sup> std. state            | aq             | - 626.22                                     | - 527.8                                      | 139.8                                                  |                                                          |
| HSO <sub>4</sub> <sup>-</sup>                       | aq             | - 886.9(10)                                  | - 755.9                                      | 131.7(30)                                              | - 84.0                                                   |
| HSO <sub>3</sub> Cl                                 | lq             | - 601.2                                      |                                              |                                                        |                                                          |
| HSO <sub>3</sub> F                                  | lq             | - 795.0                                      |                                              |                                                        |                                                          |
|                                                     | g              | - 753                                        | - 691                                        | 297                                                    | 75.24                                                    |
| H <sub>2</sub> SO <sub>3</sub> undissoc; std. state | aq             | - 608.81                                     | - 537.90                                     | 232.2                                                  |                                                          |
| H <sub>2</sub> SO <sub>4</sub>                      | lq             | - 814.0                                      | - 689.9                                      | 156.90                                                 | 138.9                                                    |
| std. state                                          | aq             | - 909.27                                     | - 744.63                                     | 20.1                                                   | 293                                                      |
| H <sub>2</sub> SO <sub>4</sub> · H <sub>2</sub> O   | lq             | - 1127.6                                     | - 950.3                                      | 211.5                                                  | 214.3                                                    |
| H <sub>2</sub> SO <sub>4</sub> · 2H <sub>2</sub> O  | lq             | - 1427.1                                     | - 1199.6                                     | 276.4                                                  | 261.5                                                    |
| H <sub>2</sub> SO <sub>4</sub> · 3H <sub>2</sub> O  | lq             | - 1720.4                                     | - 1443.9                                     | 345.4                                                  | 319.1                                                    |
| H <sub>2</sub> SO <sub>4</sub> · 4H <sub>2</sub> O  | lq             | - 2011.2                                     | - 1685.8                                     | 414.5                                                  | 386.4                                                    |
| H <sub>2</sub> S <sub>2</sub> O <sub>7</sub>        | c              | - 1273.6                                     |                                              |                                                        |                                                          |
| H <sub>2</sub> Te                                   | g              | 99.6                                         |                                              | 228.9                                                  | 35.56                                                    |
| H <sub>2</sub> WO <sub>4</sub>                      | c              | - 1131.8                                     | - 1003.9                                     | 145                                                    | 113                                                      |
| Indium                                              |                |                                              |                                              |                                                        |                                                          |
| In                                                  | c              | 0                                            | 0                                            | 57.8                                                   | 26.7                                                     |
| In <sup>3+</sup>                                    | aq             | - 105.0                                      | - 98.0                                       | - 151.0                                                |                                                          |
| InAs                                                | c              | - 58.6                                       | - 53.6                                       | 75.7                                                   | 47.78                                                    |
| InBr <sub>3</sub>                                   | c              | - 428.9                                      |                                              |                                                        |                                                          |
| InCl <sub>3</sub>                                   | c              | - 537.2                                      |                                              |                                                        |                                                          |
| InF                                                 | g              | - 203.4                                      |                                              |                                                        |                                                          |
| InH                                                 | g              | 215.5                                        | 190.3                                        | 207.53                                                 | 29.58                                                    |
| InI                                                 | c              | - 116.3                                      | - 120.5                                      | 130.0                                                  |                                                          |
| InI <sub>3</sub>                                    | c              | - 238.0                                      |                                              |                                                        |                                                          |
| InOH <sup>2+</sup>                                  | aq             | - 370.3                                      | - 313.0                                      | - 88.0                                                 |                                                          |
| In(OH) <sub>2</sub> <sup>+</sup>                    | aq             | - 619.0                                      | - 525.0                                      | 25.0                                                   |                                                          |
| In <sub>2</sub> O <sub>3</sub>                      | c              | - 925.27                                     | - 830.73                                     | 104.2                                                  | 92                                                       |
| InP                                                 | c              | - 88.7                                       | - 77.0                                       | 59.8                                                   | 45.44                                                    |
| InS                                                 | c              | - 138.1                                      | - 131.8                                      | 67                                                     |                                                          |
| In <sub>2</sub> S <sub>3</sub>                      | c              | - 427                                        | - 412.5                                      | 163.6                                                  | 118.0                                                    |
| In <sub>2</sub> Se <sub>3</sub>                     | c              | - 343                                        |                                              |                                                        |                                                          |
| InSb                                                | c              | - 30.5                                       | - 25.5                                       | 86.2                                                   | 49.5                                                     |
| Iodine                                              |                |                                              |                                              |                                                        |                                                          |
| I atomic                                            | g              | 106.76(4)                                    | 70.2                                         | 180.787(4)                                             | 20.8                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                    | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| I <sup>-</sup> std. state                    | aq             | -56.78(5)                                    | -51.59                                       | 106.45(30)                                             | -142.3                                                   |
| I <sub>2</sub>                               | c              | 0                                            | 0                                            | 116.14(30)                                             | 54.44                                                    |
|                                              | g              | 62.42(8)                                     | 19.37                                        | 260.687(5)                                             | 36.86                                                    |
| std. state                                   | aq             | 22.6                                         | 16.40                                        | 137.2                                                  |                                                          |
| I <sub>3</sub> <sup>-</sup> std. state       | aq             | -51.5                                        | -51.5                                        | 239.3                                                  |                                                          |
| IBr                                          | c              | -10.5                                        |                                              |                                                        |                                                          |
|                                              | g              | 40.8                                         | 3.7                                          | 258.8                                                  | 36.4                                                     |
| ICl                                          | c              | -35.4                                        | -14.05                                       | 97.93                                                  | 55.23                                                    |
|                                              | lq             | -23.93                                       | -13.6                                        | 135.1                                                  |                                                          |
|                                              | g              | 17.8                                         | -5.5                                         | 247.6                                                  | 35.6                                                     |
| ICl <sub>3</sub>                             | c              | -89.5                                        | -22.34                                       | 167.4                                                  |                                                          |
| IF                                           | g              | -95.7                                        | -118.5                                       | 236.3                                                  | 33.4                                                     |
| IF <sub>5</sub>                              | lq             | -864.8                                       |                                              |                                                        |                                                          |
|                                              | g              | -822.5                                       | -751.5                                       | 327.7                                                  | 99.2                                                     |
| IF <sub>7</sub>                              | g              | -961.1                                       | -835.8                                       | 347.7                                                  | 134.5                                                    |
| IO                                           | g              | 175.1                                        | 149.8                                        | 245.5                                                  | 32.9                                                     |
| IO <sup>-</sup> std. state                   | aq             | -107.5                                       | -38.5                                        | -5.4                                                   |                                                          |
| IO <sub>3</sub> <sup>-</sup> std. state      | aq             | -221.3                                       | -128.0                                       | 118.4                                                  |                                                          |
| IO <sub>4</sub> <sup>-</sup> std. state      | aq             | -151.5                                       | -58.6                                        | 222                                                    |                                                          |
| I <sub>2</sub> O <sub>5</sub>                | c              | -158.07                                      |                                              |                                                        |                                                          |
| Iridium                                      |                |                                              |                                              |                                                        |                                                          |
| Ir                                           | c              | 0                                            | 0                                            | 35.48                                                  | 25.06                                                    |
| IrCl <sub>3</sub>                            | c              | -245.6                                       | 180                                          | 113                                                    |                                                          |
| IrF <sub>6</sub>                             | c              | -579.65                                      | -461.66                                      | 247.7                                                  |                                                          |
| IrO <sub>2</sub>                             | c              | -274.1                                       |                                              | 57.3                                                   | 57.32                                                    |
| IrS <sub>2</sub>                             | c              | -138.0                                       |                                              |                                                        |                                                          |
| Iron                                         |                |                                              |                                              |                                                        |                                                          |
| Fe alpha                                     | c              | 0                                            | 0                                            | 27.32                                                  | 25.09                                                    |
| Fe <sup>2+</sup> std. state                  | aq             | -89.1                                        | -78.87                                       | -137.7                                                 |                                                          |
| Fe <sup>3+</sup> std. state                  | aq             | -48.5                                        | -4.7                                         | -315.9                                                 |                                                          |
| FeBr <sub>2</sub>                            | c              | -249.8                                       | -238.1                                       | 140.7                                                  | 80.2                                                     |
| std. state                                   | aq             | -332.2                                       | -286.81                                      | 27.2                                                   |                                                          |
| FeBr <sub>3</sub>                            | c              | -286.2                                       |                                              |                                                        |                                                          |
|                                              | aq             | -413.4                                       | -316.7                                       | -68.6                                                  |                                                          |
| Fe <sub>3</sub> C α-cementite                | c              | 25.1                                         | 20.1                                         | 104.6                                                  | 105.9                                                    |
| FeCl <sub>2</sub>                            | c              | -341.8                                       | -302.3                                       | 118.0                                                  | 76.7                                                     |
|                                              | aq             | -423.4                                       | -341.3                                       | -24.7                                                  |                                                          |
| FeCl <sub>3</sub>                            | c              | -399.4                                       | -333.9                                       | 142.34                                                 | 96.65                                                    |
| std. state                                   | aq             | -550.2                                       | -398.3                                       | -146.4                                                 |                                                          |
| Fe(CN) <sub>6</sub> <sup>3-</sup> std. state | aq             | 561.9                                        | 729.3                                        | 270.3                                                  |                                                          |
| Fe(CN) <sub>6</sub> <sup>4-</sup> std. state | aq             | 455.6                                        | 694.9                                        | 95.0                                                   |                                                          |
| FeCNS <sup>2+</sup> std. state               | aq             | 23.4                                         | 71.1                                         | -130                                                   |                                                          |
| FeCO <sub>3</sub>                            | c              | -740.6                                       | -666.7                                       | 92.9                                                   | 82.1                                                     |
| Fe(CO) <sub>5</sub>                          | lq             | -774.0                                       | -705.3                                       | 338.1                                                  | 240.6                                                    |
| FeCr <sub>2</sub> O <sub>4</sub>             | c              | -1446.0                                      | -1343.9                                      | 146.2                                                  | 133.8                                                    |
| FeF <sub>2</sub>                             | c              | -711.3                                       | -668.6                                       | 86.99                                                  | 68.12                                                    |
| std. state                                   | aq             | -754.4                                       | -636.5                                       | -165.3                                                 |                                                          |
| FeF <sub>3</sub>                             | c              | -1042                                        | -972                                         | 98                                                     | 91.0                                                     |
|                                              | aq             | -1046.4                                      | -840.9                                       | -357.3                                                 |                                                          |
| FeI <sub>2</sub>                             | c              | -113.0                                       | -111.7                                       | 167.4                                                  | 83.7                                                     |
| std. state                                   | aq             | -199.6                                       | -182.1                                       | 84.9                                                   |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| FeI <sub>3</sub>                                | aq             | −214.2                                       | −159.4                                       | 18.0                                                   |                                                          |
| FeMoO <sub>4</sub>                              | c              | −1075.0                                      | −975.0                                       | 129.3                                                  | 118.5                                                    |
| Fe <sub>2</sub> N                               | c              | −3.8                                         |                                              | 101.3                                                  | 70.0                                                     |
| Fe(NO <sub>3</sub> ) <sub>3</sub> std. state    | aq             | −670.7                                       | −338.5                                       | 123.4                                                  |                                                          |
| FeO                                             | c              | −272.0                                       | −251.4                                       | 60.75                                                  | 49.91                                                    |
| Fe <sub>2</sub> O <sub>3</sub> hematite         | c              | −824.2                                       | −742.2                                       | 87.40                                                  | 103.9                                                    |
| Fe <sub>3</sub> O <sub>4</sub> magnetite        | c              | −1118.4                                      | −1015.4                                      | 145.27                                                 | 143.4                                                    |
| FeOH <sup>+</sup> std. state                    | aq             | −324.7                                       | −277.4                                       | −29                                                    |                                                          |
| Fe(OH) <sup>2+</sup> std. state                 | aq             | −290.8                                       | −229.4                                       | −142                                                   |                                                          |
| Fe(OH) <sub>2</sub>                             | c              | −574.0                                       | −490.0                                       | 87.9                                                   | 97.1                                                     |
| Fe(OH) <sub>3</sub>                             | c              | −833                                         | −705                                         | 104.6                                                  | 101.7                                                    |
| FeS                                             | c              | −100.0                                       | −100.4                                       | 60.32                                                  | 50.52                                                    |
| FeS <sub>2</sub> marcasite                      | c              | −167.4                                       | −156.1                                       | 53.87                                                  | 62.39                                                    |
| FeS <sub>2</sub> pyrite                         | c              | −178.2                                       | −166.9                                       | 52.92                                                  | 62.12                                                    |
| FeSiO <sub>3</sub>                              | c              | −1155                                        |                                              | 87.5                                                   | 89.4                                                     |
| Fe <sub>2</sub> SiO <sub>4</sub>                | c              | −1479.9                                      | −1379.0                                      | 145.18                                                 | 132.9                                                    |
| FeSO <sub>4</sub>                               | c              | −928.4                                       | −820.8                                       | 107.5                                                  | 100.6                                                    |
| std. state                                      | aq             | −998.3                                       | −823.4                                       | −117.6                                                 |                                                          |
| Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> | c              | −2583.0                                      | −2262.7                                      | 307.5                                                  | 264.8                                                    |
| std. state                                      | aq             | −2825.0                                      | −2243.0                                      | −571.5                                                 |                                                          |
| FeTiO <sub>3</sub>                              | c              | −1246.4                                      |                                              | 105.9                                                  | 99.5                                                     |
| FeWO <sub>4</sub>                               | c              | −1155.0                                      | −1054.0                                      | 131.8                                                  | 114.4                                                    |
| Krypton                                         |                |                                              |                                              |                                                        |                                                          |
| Kr                                              | g              | 0                                            | 0                                            | 164.085(3)                                             | 20.786                                                   |
| Lanthanum                                       |                |                                              |                                              |                                                        |                                                          |
| La                                              | c              | 0                                            | 0                                            | 56.9                                                   | 27.11                                                    |
| La <sup>3+</sup>                                | aq             | −707.1                                       | 683.7                                        | −217.6                                                 | −13.0                                                    |
| LaCl <sub>3</sub>                               | c              | −1072.2                                      |                                              | 144.4                                                  | 108.8                                                    |
| std. state                                      | aq             | −1208.8                                      | −1077.4                                      | −50.0                                                  | −423.0                                                   |
| LaCl <sub>3</sub> · 7H <sub>2</sub> O           | c              | −3178.6                                      | −2713.3                                      | 462.8                                                  | 431.0                                                    |
| LaI <sub>3</sub>                                | c              | −668.9                                       |                                              |                                                        |                                                          |
| La(NO <sub>3</sub> ) <sub>3</sub>               | c              | −1254.4                                      |                                              |                                                        |                                                          |
| std. state                                      | aq             | −1329.3                                      |                                              |                                                        |                                                          |
| La <sub>2</sub> O <sub>3</sub>                  | c              | −1793.7                                      | −1705.8                                      | 127.32                                                 | 108.78                                                   |
| La <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> | c              | −3941.3                                      |                                              | 280                                                    |                                                          |
| La <sub>2</sub> Te <sub>3</sub>                 | c              | −724                                         | −714.6                                       | 231.63                                                 | 132.13                                                   |
| Lead                                            |                |                                              |                                              |                                                        |                                                          |
| Pb                                              | c              | 0                                            | 0                                            | 64.80(30)                                              | 26.84                                                    |
|                                                 | g              | 195.2(8)                                     | 162.2                                        | 175.375(5)                                             | 20.8                                                     |
| Pb <sup>2+</sup>                                | aq             | 0.92(25)                                     | −24.4                                        | 18.5(10)                                               |                                                          |
| Pb(OAc) <sub>2</sub>                            | c              | −964.4                                       |                                              |                                                        |                                                          |
| Pb(BO <sub>2</sub> ) <sub>2</sub>               | c              | −1556                                        | −1450                                        | 131                                                    | 107.1                                                    |
| PbB <sub>4</sub> O <sub>7</sub>                 | c              | −2858                                        | −2667                                        | 167                                                    | 168                                                      |
| PbBr <sub>2</sub>                               | c              | −278.7                                       | −261.9                                       | 161.5                                                  | 80.1                                                     |
|                                                 | aq             | −244.8                                       | −232.3                                       | 175.3                                                  |                                                          |
| Pb(CH <sub>3</sub> ) <sub>4</sub>               | lq             | 97.9                                         |                                              |                                                        |                                                          |
| Pb(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> | lq             | 52.7                                         |                                              | 464.6                                                  | 307.4                                                    |
| PbCl <sub>2</sub>                               | c              | −359.4                                       | −314.1                                       | 136                                                    | 77.1                                                     |
|                                                 | aq             | −336.0                                       | −286.9                                       | 123.4                                                  |                                                          |
| PbCl <sub>4</sub>                               | lq             | −329.3                                       |                                              |                                                        |                                                          |
| PbClF                                           | c              | −534.7                                       | −488.3                                       | 121.8                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| PbCO <sub>3</sub>                               | c              | -699.2                                       | -625.5                                       | 131.0                                                  | 87.40                                                    |
| PbC <sub>2</sub> O <sub>4</sub>                 | c              | -851.4                                       | -750.2                                       | 146.0                                                  | 105.4                                                    |
| PbCrO <sub>4</sub>                              | c              | -930.9                                       |                                              |                                                        |                                                          |
| PbF <sub>2</sub>                                | c              | -664                                         | -617.1                                       | 110.5                                                  | 72.3                                                     |
|                                                 | aq             | -666.9                                       | -582.0                                       | -17.2                                                  |                                                          |
| PbF <sub>4</sub>                                | c              | -941.8                                       |                                              |                                                        |                                                          |
| PbI <sub>2</sub>                                | c              | -175.5                                       | -173.58                                      | 174.9                                                  | 77.4                                                     |
|                                                 | aq             | -112.1                                       | -127.6                                       | 233.0                                                  |                                                          |
| PbMoO <sub>4</sub>                              | c              | -1051.9                                      | -951.4                                       | 166.1                                                  | 119.70                                                   |
| Pb(N <sub>3</sub> ) <sub>2</sub> monoclinic     | c              | 478.2                                        | 624.7                                        | 148.1                                                  |                                                          |
| Pb(NO <sub>3</sub> ) <sub>2</sub>               | c              | -451.9                                       |                                              |                                                        |                                                          |
|                                                 | aq             | -416.3                                       | -246.9                                       | 303.3                                                  |                                                          |
| PbO litharge                                    | c              | -219.0                                       | -188.9                                       | 66.5                                                   | 45.8                                                     |
| PbO <sub>2</sub>                                | c              | -277.4                                       | -217.3                                       | 68.60                                                  | 64.6                                                     |
| Pb <sub>3</sub> O <sub>4</sub>                  | c              | -718.4                                       | -601.2                                       | 211.3                                                  | 146.9                                                    |
| Pb <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> | c              | -2595.3                                      | -2432.6                                      | 353.1                                                  | 256.3                                                    |
| PbS                                             | c              | -100.4                                       | -98.7                                        | 91.3                                                   | 49.4                                                     |
| PbSe                                            | c              | -102.9                                       | -101.7                                       | 102.5                                                  | 50.2                                                     |
| PbSeO <sub>4</sub>                              | c              | -609.2                                       | 505.0                                        | 167.8                                                  |                                                          |
| PbSiO <sub>3</sub>                              | c              | -1145.7                                      | -1062.1                                      | 109.6                                                  | 90.04                                                    |
| PbSiO <sub>4</sub>                              | c              | -2023.8                                      | -1909.6                                      | 84.01                                                  | 98.66                                                    |
| Pb <sub>2</sub> SiO <sub>4</sub>                | c              | -1363.1                                      | -1252.6                                      | 186.6                                                  | 137.2                                                    |
| PbSO <sub>3</sub>                               | c              | -669.9                                       |                                              |                                                        |                                                          |
| PbSO <sub>4</sub>                               | c              | -919.97(40)                                  | -813.0                                       | 148.50(60)                                             | 103.2                                                    |
| PbSO <sub>4</sub> · PbO                         | c              | -1182.0                                      |                                              | 225.06                                                 | 150.16                                                   |
| PbTe                                            | c              | -70.7                                        | -69.5                                        | 110.0                                                  | 50.5                                                     |
| Lithium                                         |                |                                              |                                              |                                                        |                                                          |
| Li                                              | c              | 0                                            | 0                                            | 29.12(20)                                              | 24.8                                                     |
|                                                 | g              | 159.3(10)                                    |                                              | 138.782(10)                                            |                                                          |
| Li <sup>+</sup> std. state                      | aq             | -278.47(8)                                   | -293.30                                      | 12.24(15)                                              | 68.6                                                     |
| Li <sub>3</sub> AlF <sub>6</sub> cryolite       | c              | -3317                                        | -3152                                        | 238.5                                                  | 215.7                                                    |
| LiAlH <sub>4</sub>                              | c              | -116.3                                       | -44.7                                        | 78.7                                                   | 83.2                                                     |
| LiAlO <sub>2</sub>                              | c              | -1188.7                                      | -1126.3                                      | 53.3                                                   | 67.78                                                    |
| LiBeF <sub>3</sub>                              | c              | -1651.8                                      | -1576.3                                      | 89.2                                                   | 91.8                                                     |
| LiBH <sub>4</sub>                               | c              | -190.8                                       | -125.0                                       | 75.9                                                   | 82.6                                                     |
| LiBH <sub>4</sub> · tetrahydrofuran             | c              | -415.5                                       | -220.5                                       | 289                                                    |                                                          |
| Li <sub>2</sub> BeF <sub>4</sub>                | c              | -2274                                        | -2171                                        | 130.6                                                  | 135.3                                                    |
| LiBO <sub>2</sub>                               | c              | -1032.2                                      | -976.1                                       | 51.5                                                   | 59.8                                                     |
| Li <sub>2</sub> B <sub>4</sub> O <sub>7</sub>   | c              | -3362                                        | -3170                                        | 156                                                    | 183.0                                                    |
| LiBr                                            | c              | -351.2                                       | -342.00                                      | 74.27                                                  | 48.91                                                    |
| std. state                                      | aq             | -400.03                                      | -397.27                                      | 95.81                                                  | -73.2                                                    |
| LiBrO <sub>3</sub>                              | c              | -346.98                                      |                                              |                                                        |                                                          |
| std. state                                      | aq             | -345.56                                      | -274.89                                      | 174.9                                                  |                                                          |
| LiCl                                            | c              | -408.6                                       | -384.4                                       | 59.3                                                   | 48.03                                                    |
|                                                 | aq             | -445.6                                       | -424.6                                       | 69.9                                                   | -67.8                                                    |
| LiClO <sub>4</sub>                              | c              | -381.0                                       | -254                                         | 126                                                    | 105                                                      |
| std. state                                      | aq             | -407.81                                      | -302.1                                       | 195.4                                                  | -7.5                                                     |
| Li <sub>2</sub> CO <sub>3</sub>                 | c              | -1215.9                                      | -1132.12                                     | 90.4                                                   | 99.1                                                     |
|                                                 | aq             | -1234.1                                      | -1114.6                                      | -29.7                                                  |                                                          |
| LiF                                             | c              | -616.0                                       | -587.7                                       | 35.66                                                  | 41.6                                                     |
| std. state                                      | aq             | -611.12                                      | -571.9                                       | -0.4                                                   | -38.1                                                    |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                              | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| LiH                                                    | c              | −90.5                                        | −68.45                                       | 20.04                                                  | 27.96                                                    |
| LiI                                                    | c              | −270.4                                       | −270.3                                       | 86.8                                                   | 51.0                                                     |
| std. state                                             | aq             | −333.67                                      | −344.8                                       | 124.7                                                  | −73.6                                                    |
| LiIO <sub>3</sub>                                      | c              | −503.38                                      |                                              |                                                        |                                                          |
| std. state                                             | aq             | −499.82                                      | −421.33                                      | 131.4                                                  | −55.2                                                    |
| Li <sub>3</sub> N                                      | c              | −164.6                                       | −128.6                                       | 62.59                                                  | 75.27                                                    |
| LiNO <sub>2</sub>                                      | c              | −372.4                                       | −302.0                                       | 96.0                                                   |                                                          |
| LiNO <sub>3</sub>                                      | c              | −483.1                                       | −381.1                                       | 90.0                                                   |                                                          |
| std. state                                             | aq             | −485.9                                       | −404.5                                       | 160.2                                                  | −18.0                                                    |
| Li <sub>2</sub> O                                      | c              | −597.9                                       | −561.2                                       | 37.6                                                   |                                                          |
| Li <sub>2</sub> O <sub>2</sub>                         | c              | −634.3                                       | −578.9                                       | 56.5                                                   | 70.6                                                     |
| LiOH                                                   | c              | −484.9                                       | −439                                         | 42.82                                                  | 49.7                                                     |
| std. state                                             | aq             | −508.40                                      | −451.9                                       | 7.1                                                    |                                                          |
| Li <sub>3</sub> PO <sub>4</sub>                        | c              | −2095.8                                      |                                              |                                                        |                                                          |
| Li <sub>2</sub> SiO <sub>3</sub>                       | c              | −1648.1                                      | −1557.2                                      | 79.8                                                   | 99.1                                                     |
| Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub>         | c              | −2561                                        | −2417                                        | 125.5                                                  | 138.1                                                    |
| Li <sub>2</sub> SO <sub>4</sub>                        | c              | −1436.4                                      | −1321.7                                      | 115.1                                                  | 117.6                                                    |
| std. state                                             | aq             | −1466.2                                      | −1331.2                                      | 7.3                                                    | −155.6                                                   |
| Li <sub>2</sub> TiO <sub>3</sub>                       | c              | −1670.7                                      | −1579.8                                      | 91.8                                                   | 109.9                                                    |
| Lutetium                                               |                |                                              |                                              |                                                        |                                                          |
| Lu                                                     | c              | 0                                            | 0                                            | 50.96                                                  | 26.86                                                    |
| Lu <sup>3+</sup>                                       | aq             | −665.0                                       | −628.0                                       | −264.0                                                 | 25.0                                                     |
| LuCl <sub>3</sub>                                      | c              | −945.6                                       |                                              |                                                        |                                                          |
| std. state                                             | aq             | −1167.0                                      | −1021.0                                      | −96.0                                                  | −385.0                                                   |
| LuI <sub>3</sub>                                       | c              | −548.0                                       |                                              |                                                        |                                                          |
| Lu <sub>2</sub> O <sub>3</sub>                         | c              | −1878.2                                      | −1789.1                                      | 109.96                                                 | 101.75                                                   |
| Magnesium                                              |                |                                              |                                              |                                                        |                                                          |
| Mg                                                     | c              | 0                                            | 0                                            | 32.67(10)                                              | 24.87                                                    |
|                                                        | g              | 147.1(8)                                     |                                              | 148.648(3)                                             |                                                          |
| Mg <sup>2+</sup> std. state                            | aq             | −467.0(6)                                    | −454.8                                       | −137.(4)                                               |                                                          |
| MgAl <sub>2</sub> O <sub>4</sub>                       | c              | −2299                                        | −2177                                        | 89.0                                                   | 116.20                                                   |
| MgBr <sub>2</sub>                                      | c              | −524.3                                       | −503.8                                       | 117.2                                                  | 73.16                                                    |
| std. state                                             | aq             | −709.94                                      | −662.8                                       | 26.8                                                   |                                                          |
| MgBr <sub>2</sub> · 6H <sub>2</sub> O                  | c              | −2410.0                                      | −2056.0                                      | 397                                                    |                                                          |
| MgCl <sub>2</sub>                                      | c              | −641.3                                       | −591.8                                       | 89.63                                                  | 71.38                                                    |
| std. state                                             | aq             | −801.15                                      | −717.1                                       | −25.1                                                  |                                                          |
| MgCl <sub>2</sub> · 6H <sub>2</sub> O                  | c              | −2499.0                                      | −2115.0                                      | 315.1                                                  |                                                          |
| Mg(ClO <sub>4</sub> ) <sub>2</sub>                     | c              | −568.90                                      |                                              |                                                        |                                                          |
| std. state                                             | aq             | −725.51                                      | −472.0                                       | 225.4                                                  |                                                          |
| Mg(ClO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O | c              | −2445.6                                      | −1863.1                                      | 520.1                                                  |                                                          |
| MgCO <sub>3</sub>                                      | c              | −1095.8                                      | −1012.1                                      | 65.7                                                   | 75.51                                                    |
| MgC <sub>2</sub> O <sub>4</sub>                        | c              | −1269.0                                      |                                              |                                                        |                                                          |
| std. state                                             | aq             | −1292.0                                      | −1128.8                                      | −92.5                                                  |                                                          |
| MgF <sub>2</sub>                                       | c              | −1124.2(12)                                  | 1071.1                                       | 57.2(5)                                                | 61.5                                                     |
| Mg <sub>2</sub> Ge                                     | c              | −108.8                                       | −105.9                                       | 86.48                                                  | 69.54                                                    |
| MgH <sub>2</sub>                                       | c              | −75.3                                        | −35.9                                        | 31.1                                                   | 35.4                                                     |
| MgI <sub>2</sub>                                       | c              | −364.0                                       | −358.2                                       | 129.7                                                  | 74.8                                                     |
| std. state                                             | aq             | −577.22                                      | −558.1                                       | 84.5                                                   |                                                          |
| Mg <sub>3</sub> N <sub>2</sub>                         | c              | −461.1                                       | −400.9                                       | 87.9                                                   | 104.5                                                    |
| MgNH <sub>4</sub> PO <sub>4</sub> · 6H <sub>2</sub> O  | c              | −3681.9                                      |                                              |                                                        |                                                          |
| Mg(NO <sub>3</sub> ) <sub>2</sub>                      | c              | −790.65                                      | −589.5                                       | 164.0                                                  | 141.9                                                    |
| std. state                                             | aq             | −881.6                                       | −677.4                                       | 154.8                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                              | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|------------------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Mg(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O                  | c              | -2613.3                                      | -2080.7                                      | 452                                                    |                                                          |
| MgO microcrystal                                                       | c              | -601.6(3)                                    | -569.3                                       | 26.95(15)                                              | 37.2                                                     |
| Mg(OH) <sub>2</sub>                                                    | c              | -924.7                                       | -833.7                                       | 63.24                                                  | 77.25                                                    |
| std. state                                                             | aq             | -926.8                                       | -769.4                                       | -149.0                                                 |                                                          |
| Mg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>                        | c              | -3780.7                                      | -3538.8                                      | 189.20                                                 | 213.47                                                   |
| MgS                                                                    | c              | -346.0                                       | -341.8                                       | 50.3                                                   | 45.6                                                     |
| MgSeO <sub>4</sub>                                                     | c              | -968.51                                      |                                              |                                                        |                                                          |
| std. state                                                             | aq             | -1066.1                                      | -896.2                                       | -84.1                                                  |                                                          |
| Mg <sub>2</sub> Si                                                     | c              | -77.8                                        | -77.1                                        | 81.6                                                   | 67.9                                                     |
| MgSiO <sub>3</sub> clinoenstatite                                      | c              | -1548.9                                      | -1462.0                                      | 67.8                                                   | 81.9                                                     |
| Mg <sub>2</sub> SiO <sub>4</sub> forsterite                            | c              | -2174.0                                      | -2055.1                                      | 95.1                                                   | 118.5                                                    |
| Mg <sub>3</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> talc | c              | -5922.5                                      | -5543.0                                      | 260.7                                                  | 321.8                                                    |
| MgSO <sub>3</sub> · 3H <sub>2</sub> O                                  | c              | -1931.8                                      |                                              |                                                        |                                                          |
| MgSO <sub>3</sub> · 6H <sub>2</sub> O                                  | c              | -2817.5                                      |                                              |                                                        |                                                          |
| MgSO <sub>4</sub>                                                      | c              | -1284.9                                      | -1170.6                                      | 91.6                                                   | 96.5                                                     |
| std. state                                                             | aq             | -1376.1                                      | -1199.5                                      | -118.01                                                |                                                          |
| MgSO <sub>4</sub> · H <sub>2</sub> O kieserite                         | c              | -1602.1                                      | -1428.8                                      | 126.4                                                  |                                                          |
| MgSO <sub>4</sub> · 7H <sub>2</sub> O epsomite                         | c              | -3388.71                                     | -2871.9                                      | 372                                                    |                                                          |
| MgTiO <sub>3</sub>                                                     | c              | -1497.6                                      | -1420.1                                      | 111.08                                                 | 91.88                                                    |
| Mg <sub>2</sub> TiO <sub>4</sub>                                       | c              | -2164.0                                      | -2048                                        | 115.0                                                  | 129                                                      |
| MgTi <sub>2</sub> O <sub>5</sub>                                       | c              | -2509                                        | -2369                                        | 135.6                                                  | 146.9                                                    |
| Mg <sub>2</sub> V <sub>2</sub> O <sub>7</sub> , triclinic              | c              | -2835.9                                      | -2645.29                                     | 200.4                                                  | 203.47                                                   |
| MgWO <sub>4</sub>                                                      | c              | -1516                                        | -1404                                        | 101.2                                                  | 109.1                                                    |
| Manganese                                                              |                |                                              |                                              |                                                        |                                                          |
| Mn                                                                     | c              | 0                                            | 0                                            | 32.01                                                  | 26.30                                                    |
| Mn <sup>2+</sup> std. state                                            | aq             | -220.75                                      | -228.1                                       | -73.6                                                  | 50                                                       |
| MnBr <sub>2</sub>                                                      | c              | -384.9                                       | -372                                         | 138.1                                                  | 75.31                                                    |
| std. state                                                             | aq             | -464.0                                       | -409.2                                       |                                                        |                                                          |
| Mn <sub>3</sub> C                                                      | c              | -4.6                                         | 5.4                                          | 98.7                                                   | 93.51                                                    |
| MnCl <sub>2</sub>                                                      | c              | -481.3                                       | -440.5                                       | 118.20                                                 | 72.9                                                     |
| std. state                                                             | aq             | -555.05                                      | -490.8                                       | 38.9                                                   | -222                                                     |
| MnCO <sub>3</sub>                                                      | c              | -894.1                                       | -816.7                                       | 85.8                                                   | 81.5                                                     |
| Mn <sub>2</sub> (CO) <sub>10</sub>                                     | c              | -1677.4                                      |                                              |                                                        |                                                          |
| MnF <sub>2</sub>                                                       | c              | -795.0                                       | -749                                         | 92.26                                                  | 67.99                                                    |
| MnI <sub>2</sub>                                                       | c              | -242.7                                       |                                              | 150.6                                                  | 75.35                                                    |
| std. state                                                             | aq             | -331.0                                       |                                              |                                                        |                                                          |
| Mn(NO <sub>3</sub> ) <sub>2</sub>                                      | c              | -576.26                                      |                                              |                                                        |                                                          |
| std. state                                                             | aq             | -635.6                                       | -451.0                                       | 218.0                                                  | -121.0                                                   |
| MnO                                                                    | c              | -385.2                                       | -362.9                                       | 59.8                                                   | 45.4                                                     |
| MnO <sub>2</sub>                                                       | c              | -520.1                                       | -465.2                                       | 53.1                                                   | 54.1                                                     |
| Mn <sub>2</sub> O <sub>3</sub>                                         | c              | -959.0                                       | -881.2                                       | 110.5                                                  | 107.7                                                    |
| MnO <sub>4</sub>                                                       | aq             | -541.4                                       | -447.3                                       | 191.2                                                  | -82.0                                                    |
| MnO <sub>4</sub> <sup>2-</sup>                                         | aq             | -653.0                                       | -500.8                                       | 59                                                     |                                                          |
| Mn <sub>3</sub> O <sub>4</sub>                                         | c              | -1387.8                                      | -1283.2                                      | 155.6                                                  | 139.7                                                    |
| Mn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>                        | c              | -3116.7                                      |                                              |                                                        |                                                          |
| MnS                                                                    | c              | -214.2                                       | -218.4                                       | 78.2                                                   | 50.0                                                     |
| MnSe                                                                   | c              | -106.7                                       | -111.7                                       | 90.8                                                   | 51.0                                                     |
| MnSiO <sub>3</sub>                                                     | c              | -1320.9                                      | -1240.6                                      | 89.1                                                   | 86.4                                                     |
| MnSiO <sub>4</sub>                                                     | c              | -1730.5                                      | -1632.1                                      | 163.2                                                  | 129.9                                                    |
| MnSO <sub>4</sub>                                                      | c              | -1065.3                                      | -957.42                                      | 112.1                                                  | 100.4                                                    |
| std. state                                                             | aq             | -1130.1                                      | -972.8                                       | -53.6                                                  | -243                                                     |
| MnTiO <sub>3</sub>                                                     | c              | -1355.6                                      |                                              | 105.9                                                  | 99.8                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Mercury                                         |                |                                              |                                              |                                                        |                                                          |
| Hg                                              | lq             | 0                                            | 0                                            | 75.90(12)                                              | 28.00                                                    |
|                                                 | g              | 61.38(4)                                     | 31.8                                         | 174.971(5)                                             | 20.8                                                     |
| Hg <sup>2+</sup>                                | aq             | 170.21(20)                                   |                                              | -36.19(80)                                             |                                                          |
| Hg <sup>+</sup>                                 | aq             | 166.87(50)                                   |                                              | 65.74(80)                                              |                                                          |
| HgBr <sub>2</sub>                               | c              | -170.7                                       | -153.1                                       | 172.0                                                  | 75.3                                                     |
| Hg <sub>2</sub> Br <sub>2</sub>                 | c              | -206.9                                       | -181.1                                       | 218.0                                                  | 104.6                                                    |
| Hg(CH <sub>3</sub> ) <sub>2</sub>               | lq             | 59.8                                         | 140.2                                        | 209                                                    |                                                          |
| Hg(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> | lq             | 30.1                                         |                                              |                                                        |                                                          |
| HgCl <sub>2</sub>                               | c              | -224.3                                       | -178.6                                       | 146.0                                                  | 73.9                                                     |
| Hg <sub>2</sub> Cl <sub>2</sub>                 | c              | -265.37(40)                                  | -210.7                                       | 191.6(8)                                               | 102.0                                                    |
| Hg(CN) <sub>2</sub>                             | c              | 263.6                                        |                                              |                                                        |                                                          |
| Hg <sub>2</sub> CO <sub>3</sub>                 | c              | -553.5                                       | -468.1                                       | 180.0                                                  |                                                          |
| HgC <sub>2</sub> O <sub>4</sub>                 | c              | -678.2                                       |                                              |                                                        |                                                          |
| HgF <sub>2</sub>                                | c              | -405                                         | -362                                         | 134.3                                                  | 74.86                                                    |
| Hg <sub>2</sub> F <sub>2</sub>                  | c              | -485                                         | -469                                         | 161                                                    | 100.4                                                    |
| HgI <sub>2</sub>                                | c              | -105.4                                       | -101.7                                       | 180.0                                                  | 77.75                                                    |
| Hg <sub>2</sub> I <sub>2</sub>                  | c              | -121.3                                       | -111.1                                       | 233.5                                                  | 105.9                                                    |
| Hg <sub>2</sub> (N <sub>3</sub> ) <sub>2</sub>  | c              | 594.1                                        | 746.4                                        | 205                                                    |                                                          |
| HgO                                             | c              | -90.79(12)                                   | -58.49                                       | 70.25(30)                                              | 44.06                                                    |
| HgS                                             | c              | -58.2                                        | -50.6                                        | 82.4                                                   | 48.4                                                     |
| HgSO <sub>4</sub>                               | c              | -707.5                                       | -594                                         |                                                        |                                                          |
| Hg <sub>2</sub> SO <sub>4</sub>                 | c              | -743.09(40)                                  | -625.8                                       | 200.70(20)                                             | 131.96                                                   |
| HgTe                                            | c              | -42.0                                        |                                              |                                                        |                                                          |
| Molybdenum                                      |                |                                              |                                              |                                                        |                                                          |
| Mo                                              | c              | 0                                            | 0                                            | 28.71                                                  | 24.13                                                    |
| MoBr <sub>3</sub>                               | c              | -284                                         | -259                                         | 175                                                    | 105.4                                                    |
| MoCl <sub>4</sub>                               | c              | -477                                         | -402                                         | 224                                                    | 128                                                      |
| MoCl <sub>5</sub>                               | c              | -527                                         | -423                                         | 238                                                    | 155.6                                                    |
| MoCl <sub>6</sub>                               | c              | -523                                         | -391                                         | 255                                                    | 175                                                      |
| Mo(CO) <sub>6</sub>                             | c              | -982.8                                       | -877.8                                       | 325.9                                                  | 242.3                                                    |
| MoF <sub>6</sub>                                | lq             | -1585.66                                     | -1473.17                                     | 259.69                                                 | 169.8                                                    |
| MoO <sub>2</sub>                                | c              | -588.9                                       | -533.0                                       | 46.3                                                   | 56.0                                                     |
| MoO <sub>3</sub>                                | c              | -745.2                                       | -668.1                                       | 77.8                                                   | 75.0                                                     |
| MoO <sub>4</sub> <sup>2-</sup> std. state       | aq             | -997.9                                       | -836.4                                       | 27.2                                                   |                                                          |
| MoS <sub>2</sub>                                | c              | -235.1                                       | -225.9                                       | 62.57                                                  | 63.56                                                    |
| Mo <sub>2</sub> S <sub>3</sub>                  | c              | -270.3                                       | -278.6                                       | 181.2                                                  | 109.3                                                    |
| Neodymium                                       |                |                                              |                                              |                                                        |                                                          |
| Nd                                              | c              | 0                                            | 0                                            | 71.6                                                   | 27.5                                                     |
| Nd <sup>3+</sup> std. state                     | aq             | -696.2                                       | -671.5                                       | -206.7                                                 | -21                                                      |
| NdCl <sub>3</sub>                               | c              | -1041.0                                      |                                              |                                                        | 113                                                      |
| std. state                                      | aq             | -1197.9                                      | -1065.7                                      | -37.7                                                  | -431                                                     |
| NdF <sub>3</sub>                                | c              | -1657.0                                      |                                              |                                                        |                                                          |
| Nd(NO <sub>3</sub> ) <sub>3</sub>               | c              | -1230.9                                      |                                              |                                                        |                                                          |
| Nd <sub>2</sub> O <sub>3</sub>                  | c              | -1807.9                                      | -1720.9                                      | 158.6                                                  | 111.3                                                    |
| Neon                                            |                |                                              |                                              |                                                        |                                                          |
| Ne                                              | g              | 0                                            | 0                                            | 146.328(3)                                             | 20.786                                                   |
| Neptunium                                       |                |                                              |                                              |                                                        |                                                          |
| Np                                              | c              | 0                                            | 0                                            |                                                        | 29.46                                                    |
| NpF <sub>6</sub>                                | c              | -1937                                        |                                              |                                                        |                                                          |
| NpO <sub>2</sub>                                | c              | -1029                                        | -979                                         | 80.3                                                   | 66.1                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                    | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| <b>Nickel</b>                                |                |                                              |                                              |                                                        |                                                          |
| Ni                                           | c              | 0                                            | 0                                            | 29.87                                                  | 26.1                                                     |
| Ni <sup>2+</sup> std. state                  | aq             | -54.0                                        | -45.6                                        | -128.9                                                 |                                                          |
| Ni(OAc) <sub>2</sub> std. state              | aq             | -1025.9                                      | -784.5                                       | 44.4                                                   |                                                          |
| NiBr <sub>2</sub>                            | c              | -212.1                                       |                                              |                                                        |                                                          |
|                                              | aq             | -297.1                                       | -253.6                                       | 36.0                                                   |                                                          |
| NiCl <sub>2</sub>                            | c              | -305.3                                       | -259.0                                       | 97.7                                                   | 71.66                                                    |
| std. state                                   | aq             | -388.3                                       | -307.9                                       | -15.1                                                  |                                                          |
| Ni(CN) <sub>4</sub> <sup>2-</sup> std. state | aq             | 367.8                                        | 472.0                                        | 218                                                    |                                                          |
| Ni(CO) <sub>4</sub>                          | lq             | -633.0                                       | -588.2                                       | 313                                                    | 404.6                                                    |
|                                              | g              | -602.9                                       | -587.2                                       | 410.6                                                  | 145.2                                                    |
| NiC <sub>2</sub> O <sub>4</sub>              | c              | -856.9                                       |                                              |                                                        |                                                          |
| NiF <sub>2</sub>                             | c              | -651.5                                       | -604.2                                       | 73.6                                                   | 64.1                                                     |
|                                              | aq             | -719.2                                       | -603.3                                       | -156.5                                                 |                                                          |
| NiI <sub>2</sub>                             | c              | -78.8                                        |                                              |                                                        |                                                          |
|                                              | aq             | -164.4                                       | -149.0                                       | 93.7                                                   |                                                          |
| Ni(NO <sub>3</sub> ) <sub>2</sub>            | c              | -415.1                                       |                                              |                                                        |                                                          |
| std. state                                   | aq             | -468.6                                       | -268.6                                       | 164.0                                                  |                                                          |
| NiO                                          | c              | -240.6                                       | -211.7                                       | 38.00                                                  | 44.31                                                    |
| Ni <sub>2</sub> O <sub>3</sub>               | c              | -489.5                                       |                                              |                                                        |                                                          |
| NiOH <sup>+</sup>                            | aq             | -287.9                                       | -227.6                                       | -71.0                                                  |                                                          |
| Ni(OH) <sub>2</sub>                          | c              | -529.7                                       | -447.3                                       | 88.0                                                   |                                                          |
| NiS                                          | c              | -82.0                                        | -79.5                                        | 53.0                                                   | 47.1                                                     |
| Ni <sub>3</sub> S <sub>2</sub>               | c              | -216.0                                       | -210                                         | 133.9                                                  | 117.7                                                    |
| NiS <sub>2</sub>                             | c              | -131.4                                       | -124.7                                       | 72                                                     | 70.6                                                     |
| NiSO <sub>4</sub>                            | c              | -872.9                                       | -759.8                                       | 92.0                                                   | 138.0                                                    |
| std. state                                   | aq             | -963.2                                       | -790.3                                       | -108.8                                                 | 327.9                                                    |
| NiSO <sub>4</sub> · 7H <sub>2</sub> O        | c              | -2976.3                                      | -2462.2                                      | 378.94                                                 | 364.59                                                   |
| NiWO <sub>4</sub>                            | c              | -1128.4                                      |                                              | 118.0                                                  | 136.0                                                    |
| <b>Niobium</b>                               |                |                                              |                                              |                                                        |                                                          |
| Nb                                           | c              | 0                                            | 0                                            | 36.4                                                   | 24.67                                                    |
| NbBr <sub>5</sub>                            | c              | -556                                         | -508                                         | 258.8                                                  | 147.9                                                    |
| NbC                                          | c              | -138.9                                       | -136.8                                       | 34.98                                                  | 36.23                                                    |
| NbCl <sub>5</sub>                            | c              | -797.5                                       | -683.3                                       | 210.5                                                  | 148.1                                                    |
| NbF <sub>5</sub>                             | c              | -1813.8                                      | -1699.0                                      | 160.3                                                  | 134.7                                                    |
| NbI <sub>5</sub>                             | c              | -268.6                                       |                                              | 343                                                    | 155.6                                                    |
| NbN                                          | c              | -236.4                                       | -205.9                                       | 34.5                                                   | 39.0                                                     |
| NbO                                          | c              | -405.8                                       | -392.6                                       | 48.1                                                   | 41.3                                                     |
| NbO <sub>2</sub>                             | c              | -796.2                                       | -740.5                                       | 54.5                                                   | 57.45                                                    |
| Nb <sub>2</sub> O <sub>5</sub>               | c              | -1899.5                                      | -1765.8                                      | 137.3                                                  | 132.0                                                    |
| NbOCl <sub>3</sub>                           | c              | -879.5                                       | -782                                         | 159                                                    | 120.0                                                    |
| <b>Nitrogen</b>                              |                |                                              |                                              |                                                        |                                                          |
| N atomic                                     | g              | 472.68(40)                                   |                                              | 153.301(3)                                             |                                                          |
| N <sub>2</sub>                               | g              | 0                                            | 0                                            | 191.609(4)                                             | 29.124                                                   |
| N <sub>3</sub> <sup>-</sup>                  | aq             | 275.1                                        | 348.2                                        | 107.9                                                  |                                                          |
| NCl <sub>3</sub>                             | lq             | 230.0                                        |                                              |                                                        |                                                          |
| NF <sub>2</sub>                              | g              | 43.1                                         | 57.8                                         | 249.9                                                  | 41.0                                                     |
| NF <sub>3</sub>                              | g              | -132.1                                       | -90.6                                        | 260.8                                                  | 53.37                                                    |
| H <sub>2</sub> NOH                           | c              | -114.2                                       |                                              |                                                        |                                                          |
| N <sub>2</sub> F <sub>2</sub> <i>cis</i>     | g              | 69.5                                         | 109                                          | 259.8                                                  | 49.96                                                    |
| <i>trans</i>                                 | g              | 82.0                                         | 120.5                                        | 262.6                                                  | 53.47                                                    |



**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                      | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| N <sub>2</sub> F <sub>4</sub>                                  | g              | -8.4                                         | 79.9                                         | 301.2                                                  | 79.2                                                     |
| N <sub>2</sub> H <sub>4</sub> hydrazine                        | lq             | 50.6                                         | 149.3                                        | 121.2                                                  | 98.84                                                    |
| N <sub>2</sub> H <sub>4</sub> hydrazine- <i>d</i> <sub>4</sub> | g              | 81.6                                         | 150.9                                        | 248.86                                                 | 55.52                                                    |
| N <sub>2</sub> H <sub>5</sub> <sup>+</sup> std. state          | aq             | -7.5                                         | 82.4                                         | 151                                                    | 70.3                                                     |
| N <sub>2</sub> H <sub>5</sub> Br                               | c              | -155.6                                       |                                              |                                                        |                                                          |
| std. state                                                     | aq             | -128.9                                       | -21.8                                        | 233.1                                                  | -71.6                                                    |
| N <sub>2</sub> H <sub>5</sub> Cl                               | c              | -197.1                                       |                                              |                                                        |                                                          |
| std. state                                                     | aq             | -174.9                                       | -49.0                                        | 207.1                                                  | -66.1                                                    |
| N <sub>2</sub> H <sub>5</sub> Cl · HCl                         | c              | -367.4                                       |                                              |                                                        |                                                          |
| N <sub>2</sub> H <sub>5</sub> OH                               | lq             | -242.7                                       |                                              |                                                        |                                                          |
| undissoc; std. state                                           | aq             | -251.50                                      | -109.2                                       | 207.9                                                  | 73.2                                                     |
| N <sub>2</sub> H <sub>5</sub> NO <sub>3</sub>                  | c              | -251.58                                      |                                              |                                                        |                                                          |
| std. state                                                     | aq             | -215.10                                      | -28.91                                       | 297                                                    |                                                          |
| (N <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> SO <sub>4</sub>  | c              | -959.0                                       |                                              |                                                        |                                                          |
| std. state                                                     | aq             | -924.7                                       | -579.9                                       | 322                                                    | -151                                                     |
| NO                                                             | g              | 91.29                                        | 87.60                                        | 210.76                                                 | 29.85                                                    |
| NOBr                                                           | g              | 82.23                                        | 82.42                                        | 273.7                                                  | 45.48                                                    |
| NOCl                                                           | g              | 51.71                                        | 66.10                                        | 261.68                                                 | 44.7                                                     |
| NOF                                                            | g              | -66.5                                        | -51.0                                        | 248.02                                                 | 41.3                                                     |
| NOF <sub>3</sub>                                               | g              | -163                                         | -96                                          | 278.40                                                 | 67.86                                                    |
| NO <sub>2</sub>                                                | g              | 33.1                                         | 51.3                                         | 240.1                                                  | 37.2                                                     |
| NO <sub>2</sub> <sup>-</sup>                                   | aq             | -104.6                                       | -32.2                                        | 123.0                                                  | -97.5                                                    |
| NO <sub>2</sub> Cl                                             | g              | 12.6                                         | 54.4                                         | 272.19                                                 | 53.19                                                    |
| NO <sub>2</sub> F                                              | g              | -109                                         | -66                                          | 260.2                                                  | 49.8                                                     |
| NO <sub>3</sub>                                                | g              | 69.41                                        | 114.35                                       | 252.5                                                  | 46.9                                                     |
| NO <sub>3</sub> <sup>-</sup>                                   | aq             | -206.85(40)                                  | -111.3                                       | 146.70(40)                                             | -86.6                                                    |
| N <sub>2</sub> O                                               | g              | 81.6                                         | 103.7                                        | 220.0                                                  | 38.62                                                    |
| N <sub>2</sub> O <sub>2</sub>                                  | g              | 170.37                                       | 202.88                                       | 287.52                                                 | 63.51                                                    |
| N <sub>2</sub> O <sub>2</sub> <sup>2-</sup> hyponitrite        | aq             | -17.2                                        | 138.9                                        | 27.6                                                   |                                                          |
| N <sub>2</sub> O <sub>3</sub>                                  | g              | 86.6                                         | 142.4                                        | 314.7                                                  | 72.72                                                    |
| N <sub>2</sub> O <sub>4</sub>                                  | lq             | -19.5                                        | 97.5                                         | 209.20                                                 | 142.71                                                   |
|                                                                | g              | 11.1                                         | 99.8                                         | 304.38                                                 | 79.2                                                     |
| N <sub>2</sub> O <sub>5</sub>                                  | g              | 11.3                                         | 117.1                                        | 355.7                                                  | 95.30                                                    |
| NSF                                                            | g              |                                              |                                              | 259.8                                                  | 44.1                                                     |
| Osmium                                                         |                |                                              |                                              |                                                        |                                                          |
| Os                                                             | c              | 0                                            | 0                                            | 32.6                                                   | 24.7                                                     |
| OsCl <sub>3</sub>                                              | c              | -190.4                                       | -121                                         | 130                                                    |                                                          |
| OsCl <sub>4</sub>                                              | c              | -254.8                                       | -159                                         | 155                                                    |                                                          |
| OsF <sub>6</sub>                                               | g              |                                              |                                              | 358.1                                                  | 120.8                                                    |
| OsO <sub>4</sub>                                               | c              | -394.1                                       | -305.0                                       | 143.9                                                  |                                                          |
|                                                                | g              | -337.2                                       | -292.8                                       | 293.8                                                  | 74.1                                                     |
| Oxygen                                                         |                |                                              |                                              |                                                        |                                                          |
| O atomic                                                       | g              | 249.18(10)                                   | 231.7                                        | 161.059(3)                                             | 21.9                                                     |
| O <sub>2</sub>                                                 | g              | 0                                            | 0                                            | 205.152(5)                                             | 29.4                                                     |
| O <sub>3</sub>                                                 | g              |                                              | 142.7                                        | 163.2                                                  | 238.92                                                   |
| OF <sub>2</sub>                                                | g              | 24.5                                         | 41.8                                         | 247.5                                                  | 57.11                                                    |
| O <sub>2</sub> F <sub>2</sub>                                  | g              | 18.0                                         | 61.42                                        | 268.11                                                 | 54.06                                                    |
| OH <sup>-</sup>                                                | aq             | -230.015(40)                                 | -157.28                                      | -10.90(20)                                             | -148.5                                                   |
| Palladium                                                      |                |                                              |                                              |                                                        |                                                          |
| Pd                                                             | c              | 0                                            | 0                                            | 37.61                                                  | 25.94                                                    |
| Pd <sup>2+</sup> std. state                                    | aq             | 149.0                                        | 176.6                                        | -184.0                                                 |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                              | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| PdBr <sub>2</sub>                                      | c              | -104.2                                       |                                              |                                                        |                                                          |
| PdBr <sub>4</sub> <sup>2-</sup> std. state             | aq             | -384.9                                       | -318.0                                       | 247                                                    |                                                          |
| PdCl <sub>2</sub>                                      | c              | -171.5                                       | -125.1                                       | 105                                                    |                                                          |
| PdCl <sub>4</sub> <sup>2-</sup> std. state             | aq             | -550.2                                       | -416.7                                       | 167                                                    |                                                          |
| Pd <sub>2</sub> H                                      | c              | -19.7                                        | -5.0                                         | 91.6                                                   |                                                          |
| PdO                                                    | c              | -85.4                                        |                                              | 56.1                                                   | 31.5                                                     |
| PdS                                                    | c              | -75                                          | -67                                          | 46                                                     |                                                          |
| PdS <sub>2</sub>                                       | c              | -81.2                                        | -74.5                                        | 80                                                     |                                                          |
| Phosphorus                                             |                |                                              |                                              |                                                        |                                                          |
| P white                                                | c              | 0                                            | 0                                            | 41.09(25)                                              | 23.83                                                    |
|                                                        | g              | 316.5(10)                                    | 280.1                                        | 163.1199(3)                                            | 20.8                                                     |
| red, V                                                 | c              | -17.46                                       | -12.46                                       | 22.85                                                  | 21.19                                                    |
| P <sub>2</sub>                                         | g              | 144.0(20)                                    |                                              | 218.123(4)                                             |                                                          |
| P <sub>4</sub>                                         | g              | 58.9(3)                                      | 24.4                                         | 280.01(50)                                             | 67.16                                                    |
| PBr <sub>3</sub>                                       | lq             | -184.5                                       | -175.5                                       | 240.2                                                  |                                                          |
|                                                        | g              | -139.3                                       | -162.8                                       | 348.15                                                 | 76.02                                                    |
| PBr <sub>5</sub>                                       | c              | -269.9                                       |                                              |                                                        |                                                          |
| PCl <sub>3</sub>                                       | lq             | -319.7                                       | -272.4                                       | 217.2                                                  |                                                          |
|                                                        | g              | -227.1                                       | -267.8                                       | 311.8                                                  | 71.8                                                     |
| PCl <sub>5</sub>                                       | c              | -443.5                                       |                                              |                                                        |                                                          |
|                                                        | g              | -374.9                                       | -305.0                                       | 364.6                                                  | 112.8                                                    |
| PF <sub>3</sub>                                        | g              | -958                                         | -937                                         | 273.1                                                  | 58.69                                                    |
| PF <sub>5</sub>                                        | g              | -1594.4                                      | -1520.7                                      | 300.8                                                  | 84.8                                                     |
| PH <sub>3</sub>                                        | g              | 5.4                                          | 13.4                                         | 210.24                                                 | 37.10                                                    |
| std. state                                             | aq             | -9.50                                        | 25.31                                        | 120.1                                                  |                                                          |
| PH <sub>4</sub> Br                                     | c              | -127.6                                       | -47.7                                        | 110.0                                                  |                                                          |
| PH <sub>4</sub> Cl                                     | c              | -145.2                                       |                                              |                                                        |                                                          |
| PH <sub>4</sub> I                                      | c              | -69.9                                        | 0.8                                          | 123.0                                                  | 109.6                                                    |
| PH <sub>4</sub> OH undissoc; std. state                | aq             | -295.35                                      | -211.88                                      | 190.0                                                  |                                                          |
| PI <sub>3</sub>                                        | c              | -45.6                                        |                                              |                                                        |                                                          |
| PO <sub>2</sub>                                        | g              | -279.9                                       | -281.6                                       | 252.1                                                  | 39.5                                                     |
| PO <sub>3</sub>                                        | aq             | -977.0                                       |                                              |                                                        |                                                          |
| PO <sub>4</sub> <sup>3-</sup> std. state               | aq             | -1277.4                                      | -1018.8                                      | -220.5                                                 |                                                          |
| P <sub>2</sub> O <sub>7</sub> <sup>2-</sup> std. state | aq             | -2271.1                                      | -1919.2                                      | -117.0                                                 |                                                          |
| (P <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> dimer    | c              | -1640.1                                      |                                              |                                                        |                                                          |
| P <sub>4</sub> O <sub>10</sub>                         | c              | -3009.9                                      | -2723.3                                      | 228.78                                                 | 211.71                                                   |
| POBr <sub>3</sub>                                      | c              | -458.6                                       |                                              |                                                        |                                                          |
|                                                        | g              | -389.11                                      | -390.91                                      | -359.84                                                | 89.87                                                    |
| POCl <sub>3</sub>                                      | lq             | -597.1                                       | -520.9                                       | 222.46                                                 | 138.82                                                   |
|                                                        | g              | -558.5                                       | -512.9                                       | 325.5                                                  | 84.94                                                    |
| POClF <sub>2</sub>                                     | g              | -970.7                                       | -924.1                                       | 301.68                                                 | 68.83                                                    |
| POCl <sub>2</sub> F                                    | g              | -765.7                                       | -721.6                                       | 320.38                                                 | 79.32                                                    |
| POF <sub>3</sub>                                       | g              | -1254.0                                      | -1206                                        | 285.4                                                  | 68.82                                                    |
| PSCl <sub>3</sub>                                      | g              | -363.2                                       | -347.7                                       | 337.23                                                 | 89.83                                                    |
| PSF <sub>3</sub>                                       | g              | -1009                                        | -985                                         | 298.1                                                  | 74.55                                                    |
| P <sub>4</sub> S <sub>3</sub>                          | c              | -155                                         | -159                                         | 201                                                    | 146                                                      |
| Platinum                                               |                |                                              |                                              |                                                        |                                                          |
| Pt                                                     | c              | 0                                            | 41.63                                        | 25.87                                                  |                                                          |
| PtBr <sub>2</sub>                                      | c              | -82.0                                        |                                              |                                                        |                                                          |
| PtBr <sub>3</sub>                                      | c              | -120.9                                       |                                              |                                                        |                                                          |
| PtBr <sub>4</sub>                                      | c              | -156.5                                       |                                              |                                                        |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                  | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| PtCl <sub>2</sub>                          | c              | -123.4                                       |                                              | 117                                                    |                                                          |
| PtCl <sub>3</sub>                          | c              | -182.0                                       | -134                                         | 151                                                    |                                                          |
| PtCl <sub>4</sub>                          | c              | -3218                                        |                                              |                                                        |                                                          |
| PtCl <sub>4</sub> <sup>2-</sup>            | c              | -231.8                                       | -172                                         | 176                                                    |                                                          |
| PtCl <sub>4</sub> <sup>2-</sup> std. state | aq             | -499.2                                       | -361.5                                       | 155                                                    |                                                          |
| PtCl <sub>5</sub> <sup>-</sup> std. state  | aq             | -668.2                                       | -482.8                                       | 220.1                                                  |                                                          |
| PtF <sub>6</sub>                           | g              |                                              |                                              | 348.3                                                  | 122.8                                                    |
| PtI <sub>4</sub>                           | c              | -72.8                                        |                                              |                                                        |                                                          |
| PtS                                        | c              | -81.6                                        | -76.2                                        | 55.06                                                  | 43.39                                                    |
| PtS <sub>2</sub>                           | c              | -108.8                                       | -99.6                                        | 74.68                                                  | 65.90                                                    |
| Plutonium                                  |                |                                              |                                              |                                                        |                                                          |
| Pu                                         | c              | 0                                            | 0                                            | 51.5                                                   | 35.5                                                     |
| Pu <sup>3+</sup>                           | aq             | -579.9                                       | -587.9                                       | -163                                                   |                                                          |
| Pu <sup>4+</sup>                           | aq             | -579.9                                       | -1490                                        |                                                        |                                                          |
| PuBr <sub>3</sub>                          | c              | -831.8                                       | -804.6                                       | 192.88                                                 | 107.86                                                   |
| PuCl <sub>3</sub>                          | c              | -961.5                                       | -892.7                                       | 159.00                                                 | 102.84                                                   |
| PuCl <sub>4</sub>                          | c              | -1381                                        |                                              |                                                        |                                                          |
| PuF <sub>3</sub>                           | c              | -1552                                        | -1478.8                                      | 112.97                                                 | 96.82                                                    |
| PuF <sub>4</sub>                           | c              | -1732                                        | -1644.7                                      | 161.9                                                  | 120.8                                                    |
| PuF <sub>6</sub>                           | c              | 25.48                                        | 27.2                                         | 222.59                                                 | 167.36                                                   |
| PuH <sub>2</sub>                           | c              | -139.3                                       | -101.7                                       | 59.8                                                   | 39.0                                                     |
| PuH <sub>3</sub>                           | c              | -138                                         | -82.4                                        | 64.9                                                   | 43.2                                                     |
| PuI <sub>3</sub>                           | c              | -648.5                                       | -643.9                                       | 214.2                                                  | 111.8                                                    |
| PuO                                        | c              | -565                                         | -538.9                                       | 70.7                                                   | 51.3                                                     |
| PuO <sub>2</sub>                           | c              | -1058.1                                      | -1005.8                                      | 82.4                                                   | 68.6                                                     |
| Pu <sub>2</sub> O <sub>3</sub> beta        | c              | -1715.4                                      | -1632.3                                      | 152.3                                                  | 131.0                                                    |
| Pu(SO <sub>4</sub> ) <sub>2</sub>          | c              | -2200.8                                      | -1969.5                                      | 163.18                                                 | 181.96                                                   |
| PuS                                        | c              | -439.3                                       | -436.7                                       | 78.24                                                  | 53.97                                                    |
| Pu <sub>2</sub> S <sub>3</sub>             | c              | -989.5                                       | -985.5                                       | 192.46                                                 | 129.66                                                   |
| Polonium                                   |                |                                              |                                              |                                                        |                                                          |
| Po                                         | c              | 0                                            | 0                                            | 62.8                                                   | 26.4                                                     |
| PoO <sub>2</sub>                           | c              | -251                                         | -197                                         | 71                                                     | 61.5                                                     |
| Potassium                                  |                |                                              |                                              |                                                        |                                                          |
| K                                          | c              | 0                                            | 0                                            | 64.68(20)                                              | 29.60                                                    |
|                                            | lq             | 2.284                                        | 0.264                                        | 71.46                                                  | 32.72                                                    |
|                                            | g              | 89.0(8)                                      |                                              | 160.341(3)                                             |                                                          |
| K <sup>+</sup> std. state                  | aq             | -252.14(8)                                   | -283.26                                      | 101.20(20)                                             | 21.8                                                     |
| KOAc acetate                               | c              | -723.0                                       |                                              |                                                        |                                                          |
|                                            | aq             | -738.39                                      | -652.66                                      | 189.1                                                  | 15.5                                                     |
| KAg(CN) <sub>2</sub>                       | aq             | 18.0                                         | 22.2                                         | 297                                                    |                                                          |
| KAgCl <sub>2</sub>                         | aq             | -497.4                                       | -498.7                                       | 333.9                                                  |                                                          |
| K <sub>2</sub> AgI <sub>3</sub>            | aq             | -686.6                                       | -720.5                                       | 458.1                                                  |                                                          |
| KAlCl <sub>4</sub>                         | c              | 97                                           | -1094                                        | 197                                                    | 156.4                                                    |
| K <sub>3</sub> AlCl <sub>6</sub>           | c              | -2092.0                                      | -1938                                        | 377                                                    | 248.9                                                    |
| K <sub>3</sub> AlF <sub>6</sub>            | c              | -3358.1                                      |                                              | 284.5                                                  | 221.1                                                    |
| KAl(SO <sub>4</sub> ) <sub>2</sub>         | c              | -2470.2                                      | -2240.1                                      | 204.47                                                 | 192.92                                                   |
| K <sub>3</sub> AsO <sub>4</sub> std. state | aq             | -1645.27                                     | -1498.29                                     | 144.8                                                  |                                                          |
| KBF <sub>4</sub>                           | c              | -1887                                        | -1785                                        | 133.9                                                  | 114.48                                                   |
| std. state                                 | aq             | -1827.2                                      | -1770.3                                      | 285                                                    |                                                          |
| KBH <sub>4</sub>                           | c              | -227.4                                       | -160.2                                       | 106.31                                                 | 96.57                                                    |
| std. state                                 | aq             | -204.22                                      | -168.99                                      | 212.97                                                 |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                            | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|------------------------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| KBO <sub>2</sub>                                     | c              | −981.6                                                  | −923.4                                                  | 79.98                                                               | 66.7                                                                  |
| std. state                                           | aq             | −1024.75                                                | −962.19                                                 | 65.3                                                                |                                                                       |
| K <sub>2</sub> B <sub>4</sub> O <sub>7</sub>         | c              | −3334.2                                                 | −3136.8                                                 | 208                                                                 | 170.5                                                                 |
| KBr                                                  | c              | −393.8                                                  | −380.7                                                  | 95.9                                                                | 52.3                                                                  |
| std. state                                           | aq             | −373.92                                                 | −387.23                                                 | 184.9                                                               | −120.1                                                                |
| KBrO <sub>3</sub>                                    | c              | −360.2                                                  | −271.2                                                  | 149.2                                                               | 105.2                                                                 |
|                                                      | aq             | −319.45                                                 | −264.72                                                 | 264.22                                                              |                                                                       |
| KBrO <sub>4</sub>                                    | c              | −287.86                                                 | −174.47                                                 | 170.01                                                              | 120.2                                                                 |
| KCl                                                  | c              | −436.5                                                  | −408.5                                                  | 82.55                                                               | 51.29                                                                 |
| std. state                                           | aq             | −419.53                                                 | −414.51                                                 | 159.0                                                               | −114.6                                                                |
| KClO std. state                                      | aq             | −359.4                                                  | −320.1                                                  | 146                                                                 |                                                                       |
| KClO <sub>2</sub> std. state                         | aq             | −318.8                                                  | −266.1                                                  | 203.8                                                               |                                                                       |
| KClO <sub>3</sub>                                    | c              | −397.73                                                 | −296.31                                                 | 143.1                                                               | 100.3                                                                 |
| std. state                                           | aq             | −356.35                                                 | −291.29                                                 | 264.9                                                               |                                                                       |
| KClO <sub>4</sub>                                    | c              | −432.8                                                  | −303.1                                                  | 151.0                                                               | 112.41                                                                |
| std. state                                           | aq             | −381.71                                                 | −291.88                                                 | 284.5                                                               |                                                                       |
| KCN                                                  | c              | −113.1                                                  | −101.9                                                  | 128.52                                                              | 66.3                                                                  |
| std. state                                           | aq             | −101.7                                                  | −110.9                                                  | 196.7                                                               |                                                                       |
| K <sub>2</sub> CO <sub>3</sub>                       | c              | −1151.0                                                 | −1063.5                                                 | 155.5                                                               | 114.44                                                                |
| std. state                                           | aq             | −1181.90                                                | −1094.41                                                | 148.1                                                               |                                                                       |
| K <sub>2</sub> C <sub>2</sub> O <sub>4</sub>         | c              | −1346.0                                                 |                                                         |                                                                     |                                                                       |
|                                                      | aq             | −1329.72                                                |                                                         |                                                                     |                                                                       |
| K <sub>2</sub> CrO <sub>4</sub>                      | c              | −1403.7                                                 | −1295.8                                                 | 200.12                                                              | 145.98                                                                |
| std. state                                           | aq             | −1385.91                                                | −1294.36                                                | 255.2                                                               |                                                                       |
| K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>        | c              | −2061.5                                                 | −1882.0                                                 | 291.2                                                               | 219.2                                                                 |
| K <sub>2</sub> CuCl <sub>4</sub> · 2H <sub>2</sub> O | c              | −1707.1                                                 | −1492.9                                                 | 355.43                                                              | 253.22                                                                |
| KF                                                   | c              | −567.2                                                  | −537.8                                                  | 66.5                                                                | 48.98                                                                 |
| std. state                                           | aq             | −585.01                                                 | −562.08                                                 | 88.7                                                                | −84.9                                                                 |
| K <sub>3</sub> Fe(CN) <sub>6</sub>                   | c              | −249.8                                                  | −129.7                                                  | 426.06                                                              |                                                                       |
| std. state                                           | aq             | −139.4                                                  | −120.5                                                  | 577.8                                                               |                                                                       |
| K <sub>4</sub> Fe(CN) <sub>6</sub>                   | c              | −594.1                                                  | −453.1                                                  | 418.8                                                               | 322.2                                                                 |
| std. state                                           | aq             | −554.0                                                  | −438.11                                                 | 505.0                                                               |                                                                       |
| K formate                                            | c              | −679.73                                                 |                                                         |                                                                     |                                                                       |
| std. state                                           | aq             | −677.93                                                 | −634.3                                                  | 192                                                                 | −66.1                                                                 |
| K glycinate                                          | aq             | −722.16                                                 | −598.23                                                 | 221.8                                                               |                                                                       |
| KH                                                   | c              | −57.72                                                  | −53.01                                                  | 50.21                                                               | 37.91                                                                 |
| K <sub>2</sub> HAsO <sub>4</sub> std. state          | aq             | −1411.10                                                | −1281.22                                                | 203.3                                                               |                                                                       |
| KH <sub>2</sub> AsO <sub>4</sub>                     | c              | −1180.7                                                 | −1036.0                                                 | 155.02                                                              | 126.73                                                                |
| std. state                                           | aq             | −1161.94                                                | −1036.54                                                | 218                                                                 |                                                                       |
| KHCrO <sub>4</sub> std. state                        | aq             | −1130.5                                                 | −1048.1                                                 | 286.6                                                               |                                                                       |
| KHCO <sub>3</sub>                                    | c              | −963.2                                                  | −863.6                                                  | 115.5                                                               |                                                                       |
| std. state                                           | aq             | −944.33                                                 | −870.10                                                 | 193.7                                                               |                                                                       |
| KHC <sub>2</sub> O <sub>4</sub> std. state           | aq             | −1070.7                                                 | −981.7                                                  | 251.9                                                               |                                                                       |
| KHF <sub>2</sub>                                     | c              | −927.7                                                  | −859.7                                                  | 104.3                                                               | 76.94                                                                 |
|                                                      | aq             | −902.32                                                 | −861.40                                                 | 195.0                                                               |                                                                       |
| KHgBr <sub>3</sub>                                   | c              | −550.20                                                 |                                                         |                                                                     |                                                                       |
| std. state                                           | aq             | −545.6                                                  | −542.7                                                  | 360                                                                 |                                                                       |
| K <sub>2</sub> HgBr <sub>4</sub>                     | c              | −963.6                                                  |                                                         |                                                                     |                                                                       |
| std. state                                           | aq             | −935.5                                                  | −937.6                                                  | 515                                                                 |                                                                       |
| KHgCl <sub>3</sub>                                   | c              | −671.1                                                  |                                                         |                                                                     |                                                                       |
| std. state                                           | aq             | −641.0                                                  | −592.5                                                  | 314                                                                 |                                                                       |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                   | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| K <sub>2</sub> Hg(CN) <sub>4</sub>                          | c              | − 32.2                                       |                                              |                                                        |                                                          |
| std. state                                                  | aq             | 21.8                                         | 51.9                                         | 510                                                    |                                                          |
| K <sub>2</sub> HgI <sub>4</sub>                             | c              | − 775.0                                      |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 739.7                                      | − 778.2                                      | 565                                                    |                                                          |
| KH <sub>2</sub> PO <sub>4</sub>                             | c              | − 1568.33                                    | − 1415.95                                    | 134.85                                                 | 116.57                                                   |
| std. state                                                  | aq             | − 1548.67                                    | − 1622.85                                    | 192.9                                                  |                                                          |
| K <sub>2</sub> HPO <sub>4</sub> std. state                  | aq             | − 1796.90                                    | − 1655.78                                    | 171.5                                                  |                                                          |
| K <sub>2</sub> H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> | c              | − 2815.8                                     |                                              |                                                        |                                                          |
|                                                             | aq             | − 2783.2                                     | − 2576.9                                     | 368                                                    |                                                          |
| K <sub>3</sub> HP <sub>2</sub> O <sub>7</sub>               | aq             | − 3032.1                                     | − 2822.1                                     | 351                                                    |                                                          |
| KHS                                                         | c              | − 265.10                                     |                                              |                                                        | 75.3                                                     |
| std. state                                                  | aq             | − 269.9                                      | − 271.21                                     | 165.3                                                  |                                                          |
| KHSO <sub>3</sub>                                           | aq             | − 878.60                                     | − 811.07                                     | 242.3                                                  |                                                          |
| KHSO <sub>4</sub>                                           | c              | − 1160.6                                     | − 1131.4                                     | 138.1                                                  |                                                          |
| std. state                                                  | aq             | − 1139.72                                    | − 1039.26                                    | 234.3                                                  | − 63.0                                                   |
| KI                                                          | c              | − 327.9                                      | − 324.9                                      | 106.3                                                  | 52.9                                                     |
|                                                             | aq             | − 307.57                                     | − 334.85                                     | 213.8                                                  | − 120.5                                                  |
| KIO <sub>3</sub>                                            | c              | − 510.43                                     | − 418.4                                      | 151.46                                                 | 106.48                                                   |
|                                                             | aq             | − 473.6                                      | − 411.3                                      | 220.9                                                  |                                                          |
| KIO <sub>4</sub>                                            | c              | − 467.23                                     | − 361.41                                     | 175.7                                                  |                                                          |
|                                                             | aq             | − 403.8                                      | − 341.8                                      | 322                                                    |                                                          |
| KMnO <sub>4</sub>                                           | c              | − 837.2                                      | − 737.6                                      | 171.71                                                 | 117.6                                                    |
| K <sub>2</sub> MoO <sub>4</sub>                             | c              | − 1498.71                                    |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 1502.5                                     | − 1402.9                                     | 232.2                                                  |                                                          |
| KNH <sub>2</sub> amide                                      | c              | − 128.9                                      |                                              |                                                        |                                                          |
| KNO <sub>2</sub>                                            | c              | − 369.82                                     | − 306.60                                     | 152.09                                                 | 107.40                                                   |
| std. state                                                  | aq             | − 356.9                                      | − 315.5                                      | 225.5                                                  |                                                          |
| KNO <sub>3</sub>                                            | c              | − 494.63                                     | − 394.93                                     | 133.05                                                 | 96.4                                                     |
| std. state                                                  | aq             | − 459.74                                     | − 394.59                                     | 249.0                                                  | − 64.9                                                   |
| K <sub>2</sub> Ni(CN) <sub>4</sub> std. state               | aq             | − 136.8                                      | − 94.6                                       | 423                                                    |                                                          |
| K <sub>2</sub> O                                            | c              | − 361.5                                      | − 322.1                                      | 94.1                                                   | 83.7                                                     |
| KO <sub>2</sub>                                             | c              | − 284.9                                      | − 239.4                                      | 122.5                                                  | 77.53                                                    |
| K <sub>2</sub> O <sub>2</sub>                               | c              | − 494.1                                      | − 425.1                                      | 102.0                                                  | 110                                                      |
| KOCN cyanate                                                | c              | − 418.65                                     |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 398.3                                      | − 380.7                                      | 209.2                                                  |                                                          |
| KOH                                                         | c              | − 424.7                                      | − 378.7                                      | 78.9                                                   | 64.9                                                     |
| std. state                                                  | aq             | − 482.37                                     | − 440.53                                     | 91.6                                                   | − 126.8                                                  |
| K <sub>2</sub> PdBr <sub>4</sub>                            | c              | − 938.1                                      |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 889.5                                      | − 884.5                                      | 452                                                    |                                                          |
| K <sub>3</sub> PO <sub>4</sub>                              | c              | − 1950.2                                     |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 2034.7                                     | − 1868.6                                     | 87.9                                                   |                                                          |
| K <sub>4</sub> P <sub>2</sub> O <sub>7</sub>                | aq             | − 3280.7                                     | − 3052.2                                     | 293                                                    |                                                          |
| K <sub>2</sub> PtBr <sub>4</sub>                            | c              | − 915.0                                      |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 872.8                                      | − 828.4                                      | 326.4                                                  |                                                          |
| K <sub>2</sub> PtBr <sub>6</sub>                            | c              | − 1021.3                                     |                                              |                                                        |                                                          |
| std. state                                                  | aq             | − 975.3                                      | − 898.7                                      | 368                                                    |                                                          |
| K <sub>2</sub> PtCl <sub>4</sub>                            | c              | − 1054.4                                     |                                              |                                                        | 180.2                                                    |
| std. state                                                  | aq             | − 1003.7                                     | − 928.0                                      | 360                                                    |                                                          |
| K <sub>2</sub> PtCl <sub>6</sub>                            | c              | − 1229.3                                     | − 1078.6                                     | 333.9                                                  | 205.60                                                   |
| std. state                                                  | aq             | − 1171.8                                     | − 1049.4                                     | 424.7                                                  |                                                          |
| K <sub>2</sub> ReCl <sub>6</sub>                            | c              | − 1310.4                                     | − 1172.8                                     | 371.71                                                 | 214.68                                                   |
| std. state                                                  | aq             | − 1266.92                                    | − 1156.0                                     | 460                                                    |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                    | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| KReO <sub>4</sub>                            | c              | -1097.0                                      | -994.5                                       | 167.82                                                 | 122.55                                                   |
| std. state                                   | aq             | -1039.7                                      | -977.8                                       | 303.8                                                  | 8.4                                                      |
| K <sub>2</sub> S                             | c              | -380.7                                       | -364.0                                       | 105.0                                                  | 74.7                                                     |
| std. state                                   | aq             | -471.5                                       | -480.7                                       | 190.4                                                  |                                                          |
| K <sub>2</sub> S <sub>2</sub>                | c              | -432.2                                       |                                              |                                                        |                                                          |
|                                              | aq             | -474.5                                       | -487.0                                       | 233.5                                                  |                                                          |
| KSCN                                         | c              | -200.16                                      | -178.32                                      | 124.26                                                 | 88.53                                                    |
| std. state                                   | aq             | -175.94                                      | -190.58                                      | 246.9                                                  | -18.4                                                    |
| K <sub>2</sub> SeO <sub>3</sub>              | c              | -979.5                                       |                                              |                                                        |                                                          |
| std. state                                   | aq             | -1013.8                                      | -936.4                                       | 218.0                                                  |                                                          |
| K <sub>2</sub> SeO <sub>4</sub>              | c              | -1110.02                                     | -1002.9                                      | 222                                                    |                                                          |
| std. state                                   | aq             | -1103.7                                      | -1007.9                                      | 259.0                                                  |                                                          |
| K <sub>2</sub> SiF <sub>6</sub>              | c              | -2956.0                                      | -2798.7                                      | 225.9                                                  |                                                          |
| std. state                                   | aq             | -2893.7                                      | -2766.0                                      | 327.2                                                  |                                                          |
| K <sub>2</sub> SiO <sub>3</sub>              | c              | -1548.1                                      | -1455.7                                      | 146.1                                                  | 118.4                                                    |
| K <sub>2</sub> SnBr <sub>6</sub>             | c              | -1218.0                                      | -1160.2                                      | 443.1                                                  | 246.0                                                    |
| K <sub>2</sub> SnCl <sub>6</sub>             | c              | -1477.0                                      | -1333.0                                      | 366.5                                                  | 246.0                                                    |
| K <sub>2</sub> SO <sub>3</sub>               | c              | -1125.5                                      |                                              |                                                        |                                                          |
| std. state                                   | aq             | -1140.1                                      | -1053.1                                      | 176                                                    |                                                          |
| K <sub>2</sub> SO <sub>4</sub>               | c              | -1437.8                                      | -1321.4                                      | 175.6                                                  | 131.5                                                    |
|                                              | aq             | -1414.0                                      | -1311.1                                      | 225.1                                                  | -251.0                                                   |
| K <sub>2</sub> SO <sub>6</sub>               | c              | -1437.7                                      | -1319.6                                      | 175.5                                                  | 131.3                                                    |
| std. state                                   | aq             | -1414.02                                     | -1311.14                                     | 225.1                                                  | -251                                                     |
| K <sub>2</sub> S <sub>2</sub> O <sub>3</sub> | c              | -1173.6                                      |                                              |                                                        |                                                          |
| std. state                                   | aq             | -1156.9                                      | -1089.1                                      | 272                                                    |                                                          |
| K <sub>2</sub> S <sub>2</sub> O <sub>4</sub> | aq             | -1258.1                                      | -1166.9                                      | 297                                                    |                                                          |
| K <sub>2</sub> S <sub>2</sub> O <sub>7</sub> | c              | -1986.6                                      | -1791.6                                      | 255                                                    |                                                          |
| K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> | c              | -1916.10                                     | -1697.41                                     | 278.7                                                  | 213.2                                                    |
| std. state                                   | aq             | -1849.3                                      | -1681.6                                      | 449.4                                                  |                                                          |
| K <sub>2</sub> S <sub>4</sub> O <sub>6</sub> | c              | -1780.7                                      | -1613.43                                     | 309.66                                                 | 230.79                                                   |
| std. state                                   | aq             | -1728.8                                      | -1607.1                                      | 462.3                                                  | -24.3                                                    |
| KSO <sub>3</sub> F                           | c              | -1159.0                                      |                                              |                                                        |                                                          |
| K <sub>2</sub> UO <sub>4</sub>               | c              | -1921.3                                      |                                              |                                                        |                                                          |
| KVO <sub>4</sub>                             | c              | -1154.8                                      |                                              |                                                        |                                                          |
| std. state                                   | aq             | -1140.6                                      | -1066.9                                      | 155                                                    |                                                          |
| K <sub>2</sub> Zn(CN) <sub>4</sub>           | c              | -100.0                                       |                                              |                                                        |                                                          |
| std. state                                   | aq             | -162.3                                       | -119.7                                       | 431                                                    |                                                          |
| Praseodymium                                 |                |                                              |                                              |                                                        |                                                          |
| Pr                                           | c              | 0                                            | 0                                            | 73.2                                                   | 27.20                                                    |
| Pr <sup>3+</sup> std. state                  | aq             | -704.6                                       | -679.1                                       | -209.0                                                 | -29.0                                                    |
| Pr(OAc) <sub>3</sub> std. state              | aq             | -2147.52                                     | -1805.56                                     | 164.9                                                  |                                                          |
| PrCl <sub>3</sub>                            | c              | -1056.9                                      |                                              |                                                        | 100.0                                                    |
| std. state                                   | aq             | -1206.3                                      | -1072.8                                      | -42.0                                                  | -439.0                                                   |
| Pr(NO <sub>3</sub> ) <sub>3</sub>            | c              | -1229.3                                      |                                              |                                                        |                                                          |
| Pr <sub>2</sub> O <sub>3</sub>               | c              | -1809.6                                      |                                              |                                                        | 117.40                                                   |
| Promethium                                   |                |                                              |                                              |                                                        |                                                          |
| PmCl <sub>3</sub>                            | c              | -1054.0                                      |                                              |                                                        |                                                          |
| Protactinium                                 |                |                                              |                                              |                                                        |                                                          |
| Pa                                           | c              | 0                                            | 0                                            | 51.8                                                   |                                                          |
| Pa <sup>4+</sup>                             | aq             | -619.2                                       |                                              |                                                        |                                                          |
| PaBr <sub>4</sub>                            | c              | -824.0                                       | -787.9                                       | 234.0                                                  |                                                          |
| PaBr <sub>5</sub>                            | c              | -862                                         | -820                                         | 289                                                    |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                  | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| PaCl <sub>4</sub>                          | c              | −1043.1                                      | −953.0                                       | 192.0                                                  |                                                          |
| PaCl <sub>5</sub>                          | c              | −1144.7                                      | −1034.3                                      | 238.0                                                  |                                                          |
| Radium                                     |                |                                              |                                              |                                                        |                                                          |
| Ra                                         | c              | 0                                            | 0                                            | 71                                                     |                                                          |
| Ra <sup>2+</sup>                           | aq             | −527.6                                       | −561.5                                       | 54.0                                                   |                                                          |
| RaCl <sub>2</sub> std. state               | aq             | −861.9                                       | −823.8                                       | 167.0                                                  |                                                          |
| Ra(NO <sub>3</sub> ) <sub>2</sub>          | c              | −992                                         | −796.2                                       | 222                                                    |                                                          |
| std. state                                 | aq             | −942.2                                       | −784.1                                       | 347.0                                                  |                                                          |
| RaSO <sub>4</sub>                          | c              | −1471.1                                      | −1365.7                                      | 138                                                    |                                                          |
| std. state                                 | aq             | −1436.8                                      | −1306.2                                      | 75.0                                                   |                                                          |
| Radon                                      |                |                                              |                                              |                                                        |                                                          |
| Rn                                         | g              | 0                                            | 0                                            | 176.235                                                | 20.79                                                    |
| Rhenium                                    |                |                                              |                                              |                                                        |                                                          |
| Re                                         | c              | 0                                            | 0                                            | 36.9                                                   | 25.5                                                     |
|                                            | g              | 769.9                                        | 724.6                                        | 188.9                                                  | 20.8                                                     |
| Re <sup>−</sup> std. state                 | aq             | 46.0                                         | 10.1                                         | 230.0                                                  |                                                          |
| ReBr <sub>3</sub>                          | c              | −167.0                                       |                                              |                                                        |                                                          |
| ReCl <sub>3</sub>                          | c              | −264                                         | −188                                         | 123.9                                                  | 92.4                                                     |
| ReCl <sub>6</sub> <sup>2−</sup> std. state | aq             | −761                                         | −590                                         | 251                                                    |                                                          |
| ReO <sub>2</sub>                           | c              | −423                                         | −368                                         | 172                                                    |                                                          |
| ReO <sub>3</sub>                           | c              | −605.0                                       | −531                                         | 257.3                                                  |                                                          |
| Re <sub>2</sub> O <sub>7</sub>             | c              | −1240.1                                      | −1066.1                                      | 207.1                                                  | 166.1                                                    |
|                                            | g              | −1100.0                                      | −994.0                                       | 452.0                                                  |                                                          |
| Rhodium                                    |                |                                              |                                              |                                                        |                                                          |
| Rh                                         | c              | 0                                            | 0                                            | 31.51                                                  | 24.98                                                    |
| RhCl <sub>3</sub>                          | c              | −299.2                                       |                                              |                                                        |                                                          |
| Rh <sub>2</sub> O <sub>3</sub>             | c              | −343.0                                       |                                              | 110.9                                                  | 104.0                                                    |
| Rubidium                                   |                |                                              |                                              |                                                        |                                                          |
| Rb                                         | c              | 0                                            | 0                                            | 76.78(30)                                              | 31.06                                                    |
|                                            | g              | 80.9(8)                                      | 53.1                                         | 170.094(3)                                             | 20.8                                                     |
| Rb <sup>+</sup> std. state                 | aq             | −251.12(10)                                  | −283.97                                      | 121.75(25)                                             |                                                          |
| Rb acetate                                 | aq             | −737.2                                       | −653.3                                       | 207.9                                                  |                                                          |
| RbBO <sub>2</sub>                          | c              | −971.0                                       | −913.0                                       | 94.3                                                   | 74.1                                                     |
| RbBr                                       | c              | −394.59                                      | −381.79                                      | 109.96                                                 | 52.84                                                    |
| std. state                                 | aq             | −372.71                                      | −387.94                                      | 203.93                                                 |                                                          |
| RbBrO <sub>3</sub>                         | c              | −367.27                                      | −278.11                                      | 161.1                                                  |                                                          |
| Rb <sub>2</sub> CO <sub>3</sub>            | c              | −1136.0                                      | −1051.0                                      | 181.33                                                 | 117.61                                                   |
| std. state                                 | aq             | −1179.5                                      | −1095.8                                      | 186.2                                                  |                                                          |
| RbCl                                       | c              | −435.35                                      | −407.81                                      | 95.90                                                  | 52.41                                                    |
| std. state                                 | aq             | −418.32                                      | −415.22                                      | 178.0                                                  |                                                          |
| RbClO <sub>3</sub>                         | c              | −402.9                                       | −300.4                                       | 151.9                                                  | 103.2                                                    |
| std. state                                 | aq             | −355.14                                      | −291.9                                       | 283.68                                                 |                                                          |
| RbClO <sub>4</sub>                         | c              | −437.19                                      | −306.9                                       | 161.1                                                  |                                                          |
| std. state                                 | aq             | −380.49                                      | −292.59                                      | 303.3                                                  |                                                          |
| RbF                                        | c              | −557.7                                       |                                              | 75.3                                                   | 50.5                                                     |
| std. state                                 | aq             | −583.79                                      | −562.79                                      | 107.53                                                 |                                                          |
| Rb formate                                 | aq             | −676.7                                       | −635.1                                       | 213.0                                                  |                                                          |
| RbHCO <sub>3</sub>                         | c              | −963.2                                       | −863.6                                       | 121.3                                                  |                                                          |
| std. state                                 | aq             | −943.16                                      | −870.82                                      | 212.71                                                 |                                                          |
| RbHF <sub>2</sub>                          | c              | −922.6                                       | −855.6                                       | 120.08                                                 | 79.37                                                    |
| std. state                                 | aq             | −901.11                                      | −862.11                                      | 213.8                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|-------------------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| RbHSO <sub>4</sub>                              | c              | − 1159.0                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 1138.51                                               | − 1039.98                                               | 253.1                                                               |                                                                       |
| RbI                                             | c              | − 333.8                                                 | − 328.9                                                 | 118.4                                                               | 53.18                                                                 |
| std. state                                      | aq             | − 306.35                                                | − 335.56                                                | 232.6                                                               |                                                                       |
| RbNO <sub>2</sub>                               | c              | − 367.4                                                 | − 306.2                                                 | 172.0                                                               |                                                                       |
| RbNO <sub>3</sub>                               | c              | − 495.05                                                | − 395.85                                                | 147.3                                                               | 102.1                                                                 |
| std. state                                      | aq             | − 458.52                                                | − 395.30                                                | 267.8                                                               |                                                                       |
| Rb <sub>2</sub> O                               | c              | − 339                                                   |                                                         |                                                                     |                                                                       |
| Rb <sub>2</sub> O <sub>2</sub>                  | c              | − 472.0                                                 |                                                         |                                                                     |                                                                       |
| RbOH                                            | c              | − 418.19                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 481.16                                                | − 441.24                                                | 110.75                                                              |                                                                       |
| Rb <sub>2</sub> PtCl <sub>6</sub>               | c              | − 1245.6                                                | − 1109.6                                                | 406                                                                 |                                                                       |
| std. state                                      | aq             | − 1170.7                                                | − 1056.6                                                | 464                                                                 |                                                                       |
| RbReO <sub>4</sub>                              | c              | − 1102.9                                                | − 996.2                                                 | 167                                                                 |                                                                       |
| std. state                                      | aq             | − 1038.5                                                | − 978.6                                                 | 322.6                                                               |                                                                       |
| Rb <sub>2</sub> S                               | aq             | − 469.4                                                 | − 482.0                                                 | 228.4                                                               |                                                                       |
| Rb <sub>2</sub> SeO <sub>4</sub>                | c              | − 1114.2                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 1101.7                                                | − 1009.2                                                | 297.1                                                               |                                                                       |
| Rb <sub>2</sub> SO <sub>4</sub>                 | c              | − 1435.61                                               | − 1316.96                                               | 197.44                                                              | 134.06                                                                |
| std. state                                      | aq             | − 1411.60                                               | − 1312.56                                               | 263.2                                                               |                                                                       |
| Ruthenium                                       |                |                                                         |                                                         |                                                                     |                                                                       |
| Ru                                              | c              | 0                                                       | 0                                                       | 28.53                                                               | 24.1                                                                  |
| RuBr <sub>3</sub>                               | c              | − 138.0                                                 |                                                         |                                                                     |                                                                       |
| RuCl <sub>3</sub>                               | c              | − 205.0                                                 |                                                         |                                                                     |                                                                       |
| RuI <sub>3</sub>                                | c              | − 65.7                                                  |                                                         |                                                                     |                                                                       |
| RuO <sub>2</sub>                                | c              | − 305.0                                                 |                                                         |                                                                     |                                                                       |
| RuO <sub>4</sub>                                | c              | − 239.3                                                 | − 152.3                                                 | 146.4                                                               |                                                                       |
|                                                 | lq             | − 228.5                                                 | − 152.3                                                 | 183.3                                                               |                                                                       |
| Samarium                                        |                |                                                         |                                                         |                                                                     |                                                                       |
| Sm                                              | c              | 0                                                       | 0                                                       | 69.58                                                               | 29.54                                                                 |
| Sm <sup>3+</sup> std. state                     | aq             | − 691.6                                                 | − 666.5                                                 | − 211.7                                                             | − 21                                                                  |
| SmCl <sub>2</sub>                               | c              | − 815.5                                                 |                                                         |                                                                     |                                                                       |
| SmCl <sub>3</sub>                               | c              | − 1025.9                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 1193.3                                                | − 1060.2                                                | − 42.7                                                              | − 431                                                                 |
| SmF <sub>3</sub>                                | c              | − 1778.0                                                |                                                         |                                                                     |                                                                       |
| SmF <sub>3</sub> · ½H <sub>2</sub> O            | c              | − 1825.1                                                |                                                         |                                                                     |                                                                       |
| SmI <sub>3</sub>                                | c              | − 620.1                                                 |                                                         |                                                                     |                                                                       |
| Sm(IO <sub>3</sub> ) <sub>3</sub>               | c              | − 1381                                                  |                                                         |                                                                     |                                                                       |
| Sm(NO <sub>3</sub> ) <sub>2</sub>               | c              | − 1212.1                                                |                                                         |                                                                     |                                                                       |
| Sm <sub>2</sub> O <sub>3</sub>                  | c              | − 1823.0                                                | − 1734.7                                                | 151.0                                                               | 114.5                                                                 |
| Sm <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> | c              | − 3899.1                                                |                                                         |                                                                     |                                                                       |
| Scandium                                        |                |                                                         |                                                         |                                                                     |                                                                       |
| Sc                                              | c              | 0                                                       | 0                                                       | 34.64                                                               | 25.52                                                                 |
| Sc <sup>3+</sup> std. state                     | aq             | − 614.2                                                 | − 586.6                                                 | − 255.0                                                             |                                                                       |
| ScBr <sub>3</sub>                               | c              | − 743.1                                                 |                                                         |                                                                     |                                                                       |
| ScCl <sub>3</sub>                               | c              | − 925.1                                                 |                                                         | 121.3                                                               | 93.64                                                                 |
| ScF <sub>3</sub>                                | c              | − 1629.2                                                | − 1555.6                                                | 92                                                                  |                                                                       |
| ScOH <sup>2+</sup>                              | aq             | − 861.5                                                 | − 801.2                                                 | − 134.0                                                             |                                                                       |
| Sc <sub>2</sub> O <sub>3</sub>                  | c              | − 1908.8                                                | − 1819.41                                               | 76.99                                                               | 94.2                                                                  |



**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                 | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Selenium                                  |                |                                              |                                              |                                                        |                                                          |
| Se                                        | c              | 0                                            | 0                                            | 41.97                                                  | 24.98                                                    |
|                                           | g              | 227.1                                        | 187.0                                        | 174.8                                                  | 22.1                                                     |
| SeBr <sub>2</sub>                         | g              | -21.0                                        |                                              |                                                        |                                                          |
| SeCl <sub>4</sub>                         | c              | -188.3                                       |                                              |                                                        |                                                          |
| SeF <sub>6</sub>                          | g              | -1117.0                                      | -1017.0                                      | 313.8                                                  | 110.5                                                    |
| SeO                                       | g              | 53.4                                         | 26.8                                         | 234.0                                                  | 31.3                                                     |
| SeO <sub>2</sub>                          | c              | -225.4                                       |                                              |                                                        |                                                          |
| SeO <sub>3</sub>                          | c              | -166.9                                       |                                              |                                                        |                                                          |
| SeO <sub>3</sub> <sup>2-</sup> std. state | aq             | -509.2                                       | -369.9                                       | 13                                                     |                                                          |
| SeO <sub>4</sub> <sup>2-</sup>            | aq             | -599.2                                       | -441.4                                       | 54.0                                                   |                                                          |
| Silicon                                   |                |                                              |                                              |                                                        |                                                          |
| Si                                        | c              | 0                                            | 0                                            | 18.81(8)                                               | 20.00                                                    |
|                                           | g              | 450.(8)                                      |                                              | 167.981(4)                                             |                                                          |
| SiBr <sub>4</sub>                         | lq             | -457.3                                       | -433.9                                       | 277.5                                                  | 146.4                                                    |
|                                           | g              | -415.5                                       | -431.8                                       | 377.9                                                  | 97.1                                                     |
| SiBrCl <sub>3</sub>                       | g              |                                              |                                              | 350.1                                                  | 90.9                                                     |
| SiC alpha                                 | c              | -62.8                                        | -60.2                                        | 16.49                                                  | 26.76                                                    |
| beta                                      | c              | -65.3                                        | -62.8                                        | 16.61                                                  | 26.9                                                     |
| SiCl <sub>4</sub>                         | lq             | -686.93                                      | -620.0                                       | 239.7                                                  | 145.3                                                    |
|                                           | g              | -657.0                                       | -617.0                                       | 330.7                                                  | 90.26                                                    |
| SiClBr <sub>3</sub>                       | g              |                                              |                                              | 377.1                                                  | 95.3                                                     |
| SiClF <sub>3</sub>                        | g              | -1318                                        | -1280                                        | 309                                                    | 79.4                                                     |
| SiF <sub>4</sub>                          | g              | -1615.0(8)                                   | -1572.7                                      | 282.76(50)                                             | 73.62                                                    |
| SiH <sub>4</sub>                          | g              | 34.3                                         | 56.8                                         | 204.65                                                 | 42.83                                                    |
| SiHBr <sub>3</sub>                        | g              | -317.6                                       | -328.5                                       | 348.6                                                  | 80.8                                                     |
| SiHCl <sub>3</sub>                        | lq             | -539.3                                       | -482.5                                       | 227.6                                                  |                                                          |
|                                           | g              | -513.0                                       | -482.0                                       | 313.7                                                  | 75.8                                                     |
| SiHF <sub>3</sub>                         | g              |                                              |                                              | 271.9                                                  | 60.5                                                     |
| SiH <sub>2</sub> Cl <sub>2</sub>          | g              | -320.5                                       | -295.0                                       | 285.7                                                  | 60.5                                                     |
| SiH <sub>3</sub> Cl                       | g              | -142                                         | -119                                         | 250.8                                                  | 51.10                                                    |
| SiH <sub>3</sub> F                        | g              | -377                                         | -353                                         | 238.4                                                  | 47.20                                                    |
| Si <sub>2</sub> H <sub>6</sub>            | g              | 80.3                                         | 127.2                                        | 272.7                                                  | 80.79                                                    |
| SiI <sub>4</sub>                          | c              | -189.5                                       | -191.6                                       | 258.1                                                  | 108.0                                                    |
|                                           | lq             | -174.60                                      | -187.49                                      | 294.30                                                 | 159.79                                                   |
| Si <sub>3</sub> N <sub>4</sub>            | c              | -743.5                                       | -642.1                                       | 101.3                                                  | 99.5                                                     |
| SiO                                       | g              | -99.6                                        | -126.4                                       | 211.6                                                  | 29.9                                                     |
| SiO <sub>2</sub> quartz                   | c              | -910.7(10)                                   | -856.4                                       | 41.46(20)                                              | 44.4                                                     |
| high cristobalite                         | c              | -905.5                                       | -853.6                                       | 50.05                                                  | 26.58                                                    |
| SiOF <sub>2</sub>                         | g              | -967                                         | -951                                         | 271.3                                                  | 53.69                                                    |
| SiS <sub>2</sub>                          | c              | -213.4                                       | -212.6                                       | 80.3                                                   | 77.5                                                     |
| Silver                                    |                |                                              |                                              |                                                        |                                                          |
| Ag                                        | c              | 0                                            | 0                                            | 42.55(20)                                              | 25.4                                                     |
|                                           | g              | 284.9(8)                                     |                                              | 172.997(4)                                             |                                                          |
| Ag <sup>+</sup> std. state                | aq             | 105.79(8)                                    | 77.12                                        | 73.45(40)                                              | 21.8                                                     |
| Ag <sup>2+</sup> in 4M HClO <sub>4</sub>  | aq             | 268.6                                        | 269.0                                        | -88                                                    |                                                          |
| AgAt                                      | c              | -45.2                                        |                                              | 133.1                                                  | 55.7                                                     |
| AgBr                                      | c              | -100.37                                      | -96.90                                       | 107.11                                                 | 52.38                                                    |
| AgBrO <sub>3</sub>                        | c              | -10.5                                        | 71.3                                         | 151.9                                                  |                                                          |
| AgCl                                      | c              | -127.01(5)                                   | -109.8                                       | 96.25(20)                                              | 50.79                                                    |
| AgClO <sub>2</sub>                        | c              | 8.79                                         | 75.7                                         | 134.56                                                 | 87.32                                                    |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                 | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-----------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| AgClO <sub>3</sub>                                        | c              | -30.3                                        | 64.5                                         | 142.0                                                  |                                                          |
| AgClO <sub>4</sub>                                        | c              | -31.13                                       |                                              | 162.3                                                  |                                                          |
| std. state                                                | aq             | -23.77                                       | 68.49                                        | 254.8                                                  |                                                          |
| AgCN                                                      | c              | 146.0                                        | 156.9                                        | 107.19                                                 | 66.73                                                    |
| Ag(CN) <sub>2</sub> <sup>-</sup> std. state               | aq             | 270.3                                        | 305.4                                        | 192                                                    |                                                          |
| Ag <sub>2</sub> CrO <sub>4</sub>                          | c              | -731.74                                      | -641.83                                      | 217.6                                                  | 142.26                                                   |
| Ag <sub>2</sub> CO <sub>3</sub>                           | c              | -505.9                                       | -436.8                                       | 167.4                                                  | 112.26                                                   |
| Ag <sub>2</sub> C <sub>2</sub> O <sub>4</sub>             | c              | -673.2                                       | -584.1                                       | 209                                                    |                                                          |
| AgF                                                       | c              | -204.6                                       |                                              | 83.7                                                   | 51.92                                                    |
| AgF <sub>2</sub>                                          | c              | -360.0                                       |                                              |                                                        |                                                          |
| AgI                                                       | c              | -61.84                                       | -66.19                                       | 115.5                                                  | 56.82                                                    |
| AgIO <sub>3</sub>                                         | c              | -171.1                                       | -93.7                                        | 149.4                                                  | 102.93                                                   |
| AgN <sub>3</sub>                                          | c              | 308.8                                        | 376.1                                        | 104.2                                                  |                                                          |
| Ag(NH <sub>3</sub> ) <sub>2</sub> <sup>+</sup> std. state | aq             | -111.29                                      | -17.24                                       | 245.2                                                  |                                                          |
| AgNO <sub>3</sub>                                         | c              | -124.4                                       | -33.47                                       | 140.92                                                 | 93.05                                                    |
| std. state                                                | aq             | -101.80                                      | -34.23                                       | 219.2                                                  | -64.9                                                    |
| AgO                                                       | c              | -12.15                                       | 13.83                                        | 58.5                                                   | 44.0                                                     |
| Ag <sub>2</sub> O                                         | c              | -31.1                                        | -11.21                                       | 121.3                                                  | 65.86                                                    |
| Ag <sub>2</sub> O <sub>3</sub>                            | c              | 33.9                                         | 121.4                                        | 100.0                                                  |                                                          |
| Ag <sub>2</sub> S argentite                               | c              | -32.59                                       | -40.67                                       | 143.9                                                  | 76.53                                                    |
| Ag <sub>3</sub> Sb                                        | c              | -23.0                                        |                                              | 171.5                                                  | 101.7                                                    |
| AgSCN                                                     | c              | 87.9                                         | 101.38                                       | 131.0                                                  | 63                                                       |
| Ag <sub>2</sub> Se                                        | c              | -38                                          | -44.4                                        | 150.71                                                 | 81.76                                                    |
| Ag <sub>2</sub> SO <sub>4</sub>                           | c              | -715.9                                       | -618.4                                       | 200.4                                                  | 131.4                                                    |
| std. state                                                | aq             | -698.10                                      | -590.36                                      | 165.7                                                  | -251                                                     |
| Ag <sub>2</sub> Te                                        | c              | -37.2                                        | -43.1                                        | 154.8                                                  | 87.5                                                     |
| Sodium                                                    |                |                                              |                                              |                                                        |                                                          |
| Na                                                        | c              | 0                                            | 0                                            | 51.30(20)                                              | 28.15                                                    |
|                                                           | g              | 107.5(7)                                     |                                              | 153.718(3)                                             |                                                          |
| Na <sup>+</sup> std. state                                | aq             | -240.34(6)                                   | -261.88                                      | 58.45(15)                                              | 46.4                                                     |
| NaAg(CN) <sub>2</sub> std. state                          | aq             | 30.12                                        | 43.5                                         | 251                                                    |                                                          |
| NaOAc                                                     | c              | -708.81                                      | -607.27                                      | 123.0                                                  | 79.9                                                     |
| std. state                                                | aq             | -726.13                                      | -631.28                                      | 145.6                                                  | 40.2                                                     |
| NaAlCl <sub>4</sub>                                       | c              | -1142.0                                      | -996.4                                       | 188.3                                                  | 154.98                                                   |
| Na <sub>3</sub> AlCl <sub>6</sub>                         | c              | -1979.0                                      | -1829                                        | 347.0                                                  | 244.1                                                    |
| NaAlF <sub>4</sub>                                        | g              | -1869.0                                      | -1827.5                                      | 345.7                                                  | 105.9                                                    |
| Na <sub>3</sub> AlF <sub>6</sub>                          | c              | -3361.2                                      | -3136.7                                      | 239.5                                                  | 215.89                                                   |
| NaAlH <sub>4</sub>                                        | c              | -115.5                                       |                                              |                                                        |                                                          |
| NaAlO <sub>2</sub>                                        | c              | -1137.3                                      | -1069.2                                      | 70.40                                                  | 73.64                                                    |
| NaAl(SO <sub>4</sub> ) <sub>2</sub> std. state            | aq             | -2590                                        | -2238                                        | -222.6                                                 |                                                          |
| NaAlSiO <sub>4</sub>                                      | c              | -2092.8                                      | -1978.2                                      | 124.3                                                  |                                                          |
| NaAsO <sub>2</sub>                                        | c              | -660.53                                      |                                              |                                                        |                                                          |
| std. state                                                | aq             | -669.15                                      | -611.91                                      | 99.6                                                   |                                                          |
| Na <sub>3</sub> AsO <sub>4</sub>                          | c              | -1540                                        |                                              |                                                        |                                                          |
| std. state                                                | aq             | -1608.50                                     | -1434.19                                     | 14.2                                                   |                                                          |
| NaAu(CN) <sub>2</sub>                                     | aq             | 2.1                                          | 23.9                                         | 230                                                    |                                                          |
| NaBF <sub>4</sub>                                         | c              | -1844.7                                      | -1750.1                                      | 145.31                                                 | 120.3                                                    |
| std. state                                                | aq             | -1812.1                                      | -1748.9                                      | 243                                                    |                                                          |
| NaBH <sub>4</sub>                                         | c              | -188.6                                       | -123.9                                       | 101.3                                                  | 86.8                                                     |
| std. state                                                | aq             | -199.60                                      | -147.61                                      | 169.5                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                          | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| NaBO <sub>2</sub>                                                  | c              | −977.0                                       | −920.7                                       | 73.54                                                  | 65.94                                                    |
| std. state                                                         | aq             | −1012.49                                     | −940.81                                      | 21.8                                                   |                                                          |
| NaBO <sub>2</sub> · 4H <sub>2</sub> O                              | c              | −2114.2                                      |                                              |                                                        |                                                          |
| Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                      | c              | −3291.1                                      | −3096.0                                      | 189.0                                                  | 186.8                                                    |
| std. state                                                         | aq             | −3271.1                                      | −3076.9                                      | 192.9                                                  |                                                          |
| Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> · 10H <sub>2</sub> O | c              | −6298.6                                      | −5516.6                                      | 586                                                    | 614.5                                                    |
| NaBr                                                               | c              | −361.08                                      | −349.00                                      | 86.82                                                  | 51.38                                                    |
| std. state                                                         | aq             | −361.66                                      | −365.85                                      | 141.4                                                  | −95.4                                                    |
| NaBr <sub>3</sub> std. state                                       | aq             | −370.54                                      | −368.95                                      | 274.5                                                  |                                                          |
| NaBrO std. state                                                   | aq             | −384.3                                       | −295.4                                       | 100                                                    |                                                          |
| NaBrO <sub>3</sub>                                                 | c              | −334.09                                      | −242.6                                       | 128.9                                                  |                                                          |
| std. state                                                         | aq             | −307.19                                      | −243.34                                      | 220.9                                                  |                                                          |
| NaBrO <sub>4</sub> std. state                                      | aq             | −227.19                                      | −143.93                                      | −258.57                                                |                                                          |
| Na <sub>2</sub> [Cd(CN) <sub>4</sub> ]                             | aq             | −52.3                                        | −16.3                                        | 439                                                    |                                                          |
| NaCl                                                               | c              | −411.2                                       | −384.1                                       | 72.1                                                   | 50.51                                                    |
| std. state                                                         | aq             | −407.27                                      | −393.17                                      | 115.5                                                  | −90.0                                                    |
| NaClO std. state                                                   | aq             | −347.3                                       | −298.7                                       | 100                                                    |                                                          |
| NaClO <sub>2</sub>                                                 | c              | −307.02                                      |                                              | 115.9                                                  |                                                          |
| std. state                                                         | aq             | −306.7                                       | −244.8                                       | 160.3                                                  |                                                          |
| NaClO <sub>3</sub>                                                 | c              | −365.77                                      | −262.34                                      | 123.4                                                  |                                                          |
| std. state                                                         | aq             | −344.09                                      | −269.91                                      | 221.3                                                  |                                                          |
| NaClO <sub>4</sub>                                                 | c              | −383.3                                       | −254.9                                       | 142.3                                                  | 111.3                                                    |
| std. state                                                         | aq             | −369.45                                      | −270.50                                      | 241.0                                                  |                                                          |
| NaCN                                                               | c              | −87.5                                        | −76.4                                        | 115.6                                                  | 70.4                                                     |
| std. state                                                         | aq             | −89.5                                        | −89.5                                        | 153.1                                                  |                                                          |
| Na <sub>3</sub> [Co(NO <sub>2</sub> ) <sub>6</sub> ]               | c              | −1423.0                                      |                                              |                                                        |                                                          |
| Na <sub>2</sub> CO <sub>3</sub>                                    | c              | −1130.7                                      | −1044.4                                      | 135.0                                                  | 112.3                                                    |
|                                                                    | aq             | −1157.4                                      | −1051.6                                      | 61.6                                                   |                                                          |
| Na <sub>2</sub> CO <sub>3</sub> · H <sub>2</sub> O                 | c              | −1431.26                                     | −1285.41                                     | 168.11                                                 | 145.60                                                   |
| Na <sub>2</sub> CO <sub>3</sub> · 10H <sub>2</sub> O               | c              | −4081.32                                     | −3428.20                                     | 564.0                                                  | 550.32                                                   |
| Na <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                      | c              | −1318.0                                      |                                              |                                                        | 142                                                      |
| std. state                                                         | aq             | −1305.4                                      | −1197.9                                      | 163.6                                                  |                                                          |
| Na <sub>2</sub> CrO <sub>4</sub>                                   | c              | −1342.2                                      | −1235.0                                      | 176.61                                                 | 142.13                                                   |
| std. state                                                         | aq             | −1361.39                                     | −1251.64                                     | 168.2                                                  |                                                          |
| Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>                     | c              | −1978.6                                      |                                              |                                                        |                                                          |
| std. state                                                         | aq             | −1970.7                                      | −1825.1                                      | 379.9                                                  |                                                          |
| Na ethoxide                                                        | c              | −413.80                                      |                                              |                                                        |                                                          |
| NaF                                                                | c              | −576.6                                       | −546.3                                       | 51.11                                                  | 46.85                                                    |
| std. state                                                         | aq             | −572.75                                      | −540.70                                      | 45.2                                                   | −60.3                                                    |
| Na <sub>3</sub> [Fe(CN) <sub>6</sub> ] std. state                  | aq             | −158.6                                       | −56.5                                        | 447.3                                                  |                                                          |
| Na <sub>4</sub> [Fe(CN) <sub>6</sub> ] std. state                  | aq             | −505.0                                       | −352.63                                      | 231.0                                                  |                                                          |
| Na formate                                                         | c              | −666.5                                       | −600.00                                      | 103.76                                                 | 82.68                                                    |
| std. state                                                         | aq             | −666.67                                      | −613.0                                       | 151                                                    | −41.4                                                    |
| NaH                                                                | c              | −56.34                                       | −33.55                                       | 40.02                                                  | 36.39                                                    |
| Na <sub>2</sub> HAsO <sub>4</sub> std. state                       | aq             | −1386.58                                     | −1238.51                                     | 116.3                                                  |                                                          |
| NaH <sub>2</sub> AsO <sub>4</sub> std. state                       | aq             | −1149.68                                     | −1015.16                                     | 176                                                    |                                                          |
| NaHCO <sub>3</sub>                                                 | c              | −950.81                                      | −851.0                                       | 101.7                                                  | 87.61                                                    |
| std. state                                                         | aq             | −932.11                                      | −848.72                                      | 150.2                                                  |                                                          |
| NaHCrO <sub>4</sub> std. state                                     | aq             | −1118.4                                      | −1026.8                                      | 243.1                                                  |                                                          |
| NaHF <sub>2</sub>                                                  | c              | −920.27                                      | −852.20                                      | 90.92                                                  | 75.02                                                    |
| std. state                                                         | aq             | −890.06                                      | −840.02                                      | 151.5                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|-------------------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| $\text{Na}_2\text{H}_2[\text{Fe}(\text{CN})_6]$ | aq             | − 24.7                                                  | 134.64                                                  | 335                                                                 |                                                                       |
| $\text{NaH}_2\text{PO}_4$                       | c              | − 1536.8                                                | − 1386.2                                                | 127.49                                                              | 116.86                                                                |
| std. state                                      | aq             | − 1536.4                                                | − 1392.27                                               | 149.4                                                               |                                                                       |
| $\text{Na}_2\text{HPO}_4$                       | c              | − 1748.1                                                | − 1608.3                                                | 150.50                                                              | 135.31                                                                |
| std. state                                      | aq             | − 1772.38                                               | − 1613.06                                               | 84.5                                                                |                                                                       |
| $\text{Na}_2\text{H}_2\text{P}_2\text{O}_7$     | c              | − 2764.8                                                | − 2522.5                                                | 220.20                                                              | 198.15                                                                |
| $\text{NaHS}$                                   | c              | − 237.23                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 257.73                                                | − 249.83                                                | 121.8                                                               |                                                                       |
| $\text{NaHSeO}_3$                               | c              | − 759.23                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 754.67                                                | − 673.41                                                | 194.1                                                               |                                                                       |
| $\text{NaHSeO}_4$                               | c              | − 821.40                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 821.74                                                | − 714.2                                                 | 208.4                                                               |                                                                       |
| $\text{NaHSO}_4$                                | c              | − 1125.5                                                | − 992.9                                                 | 113.0                                                               |                                                                       |
| std. state                                      | aq             | − 1127.46                                               | − 1017.88                                               | 190.8                                                               | − 38                                                                  |
| $\text{NaI}$                                    | c              | − 287.9                                                 | − 286.1                                                 | 98.50                                                               | 52.1                                                                  |
| std. state                                      | aq             | − 295.31                                                | − 313.47                                                | 170.3                                                               | − 95.8                                                                |
| $\text{NaI}_3$                                  | aq             | − 291.6                                                 | − 313.4                                                 | 298.3                                                               |                                                                       |
| $\text{NaIO}_3$                                 | c              | − 481.79                                                |                                                         | 135.1                                                               | 92.1                                                                  |
| std. state                                      | aq             | − 461.50                                                | − 389.95                                                | 177.4                                                               |                                                                       |
| $\text{NaIO}_4$                                 | c              | − 429.28                                                | − 323.09                                                | 163.0                                                               |                                                                       |
| std. state                                      | aq             | − 391.62                                                | − 320.49                                                | 280                                                                 |                                                                       |
| $\text{Na methoxide}$                           | c              | − 367.8                                                 | − 294.80                                                | 110.58                                                              | 69.45                                                                 |
| std. state                                      | aq             | − 433.59                                                | − 332.46                                                | 17.6                                                                |                                                                       |
| $\text{NaMnO}_4$ std. state                     | aq             | − 781.6                                                 | − 709.2                                                 | 250.2                                                               |                                                                       |
| $\text{Na}_2\text{MnO}_4$                       | c              | − 1156.0                                                |                                                         |                                                                     |                                                                       |
| std. state                                      | aq             | − 1134                                                  | − 1024.7                                                | 176                                                                 |                                                                       |
| $\text{Na}_2\text{MoO}_4$                       | c              | − 1468.12                                               | − 1354.30                                               | 159.70                                                              | 141.71                                                                |
| std. state                                      | aq             | − 1478.2                                                | − 1360.2                                                | 145.2                                                               |                                                                       |
| $\text{Na}_2\text{Mo}_2\text{O}_7$              | c              | − 2245.05                                               | − 2058.19                                               | 250.6                                                               | 217.15                                                                |
| $\text{NaN}_3$                                  | c              | 21.71                                                   | 93.76                                                   | 96.86                                                               | 76.61                                                                 |
| std. state                                      | aq             | 35.02                                                   | 86.2                                                    | 166.9                                                               |                                                                       |
| $\text{NaNH}_2$                                 | c              | − 123.9                                                 | − 64.0                                                  | 76.90                                                               | 66.15                                                                 |
| $\text{NaNbO}_3$                                | c              | − 1315.9                                                | 1233.0                                                  | 117                                                                 |                                                                       |
| std. state                                      | aq             | − 1265.7                                                | − 1194.1                                                | 155                                                                 |                                                                       |
| $\text{NaNO}_2$                                 | c              | − 358.65                                                | − 284.60                                                | 103.8                                                               |                                                                       |
| std. state                                      | aq             | − 344.8                                                 | − 294.1                                                 | 182.0                                                               | − 51.0                                                                |
| $\text{NaNO}_3$                                 | c              | − 467.85                                                | − 367.06                                                | 116.52                                                              | 92.88                                                                 |
| std. state                                      | aq             | − 447.48                                                | − 373.21                                                | 205.4                                                               | − 40.2                                                                |
| $\text{Na}_2[\text{Ni}(\text{CN})_4]$           | aq             | − 112.6                                                 | − 51.9                                                  | 335                                                                 |                                                                       |
| $\text{NaO}_2$                                  | c              | − 260.2                                                 | − 218.4                                                 | 115.9                                                               | 72.14                                                                 |
| $\text{Na}_2\text{O}$                           | c              | − 414.2                                                 | − 375.5                                                 | 75.04                                                               | 69.10                                                                 |
| $\text{Na}_2\text{O}_2$                         | c              | − 510.9                                                 | − 449.6                                                 | 94.8                                                                | 89.3                                                                  |
| $\text{NaOCN cyanate}$                          | c              | − 405.39                                                | − 358.2                                                 | 96.7                                                                | 86.6                                                                  |
| std. state                                      | aq             | − 386.2                                                 | − 359.4                                                 | 165.7                                                               |                                                                       |
| $\text{NaOH}$                                   | c              | − 425.6                                                 | − 379.4                                                 | 64.4                                                                | 59.5                                                                  |
| std. state                                      | aq             | − 469.15                                                | − 419.20                                                | 48.1                                                                | − 102.1                                                               |
| $\text{Na}_3\text{PO}_4$                        | c              | − 1917.40                                               | − 1788.87                                               | 173.80                                                              | 153.47                                                                |
| std. state                                      | aq             | − 1997.9                                                | − 1804.6                                                | − 46                                                                |                                                                       |
| $\text{Na}_4\text{P}_2\text{O}_7$               | c              | − 3188                                                  | − 2969.4                                                | 270.29                                                              | 241.12                                                                |
| std. state                                      | aq             | − 3231.7                                                | − 2966.9                                                | 117                                                                 |                                                                       |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                         | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-------------------------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| NaReO <sub>4</sub>                                                | c              | −1057.09                                     | −953.74                                      | 151.5                                                  | 133.89                                                   |
| std. state                                                        | aq             | −1027.6                                      | −956.5                                       | 260.2                                                  |                                                          |
| Na <sub>2</sub> S                                                 | c              | −364.8                                       | −349.8                                       | 83.7                                                   | 82.8                                                     |
| std. state                                                        | aq             | −443.3                                       | −438.1                                       | 103.3                                                  |                                                          |
| Na <sub>2</sub> S <sub>2</sub>                                    | c              | −397.0                                       | −392                                         | 151                                                    |                                                          |
| std. state                                                        | aq             | −450.2                                       | −444.3                                       | 146.4                                                  |                                                          |
| NaSCN                                                             | c              | −170.50                                      |                                              |                                                        |                                                          |
| std. state                                                        | aq             | −163.68                                      | −169.20                                      | 203.84                                                 | 6.3                                                      |
| Na <sub>2</sub> Se                                                | c              | −341.4                                       |                                              |                                                        |                                                          |
| Na <sub>2</sub> SeO <sub>3</sub>                                  | c              | −958.6                                       |                                              |                                                        |                                                          |
| std. state                                                        | aq             | −989.5                                       | −893.7                                       | 130                                                    |                                                          |
| Na <sub>2</sub> SeO <sub>4</sub>                                  | c              | −1069.0                                      |                                              |                                                        |                                                          |
| Na <sub>2</sub> SiF <sub>6</sub>                                  | c              | −2909.6                                      | −2754.2                                      | 207.1                                                  | 187.1                                                    |
| Na <sub>2</sub> SiO <sub>3</sub>                                  | c              | −1554.9                                      | −1462.8                                      | 113.8                                                  | 111.9                                                    |
| Na <sub>2</sub> Si <sub>3</sub> O <sub>5</sub>                    | c              | −2470.1                                      | −2324.1                                      | 164.1                                                  | 157.0                                                    |
| NaSnBr <sub>3</sub>                                               | aq             | −615.1                                       | −608.8                                       | 310                                                    |                                                          |
| NaSnCl <sub>3</sub>                                               | aq             | −727.2                                       | −692.0                                       | 318                                                    |                                                          |
| Na <sub>2</sub> SO <sub>3</sub>                                   | c              | −1100.8                                      | −1012.5                                      | 145.94                                                 | 120.25                                                   |
| std. state                                                        | aq             | −1115.87                                     | −1010.44                                     | 87.9                                                   |                                                          |
| Na <sub>2</sub> SO <sub>4</sub>                                   | c              | −1387.1                                      | −1270.2                                      | 149.6                                                  | 128.2                                                    |
| std. state                                                        | aq             | −1389.51                                     | −1268.40                                     | 138.1                                                  | −201                                                     |
| Na <sub>2</sub> SO <sub>4</sub> · 10H <sub>2</sub> O              | c              | −4327.26                                     | −3647.40                                     | 592.0                                                  |                                                          |
| Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub>                     | c              | −1123.0                                      | −1028.0                                      | 155                                                    |                                                          |
| std. state                                                        | aq             | −1132.40                                     | −1046.0                                      | 184.1                                                  |                                                          |
| Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> · 5H <sub>2</sub> O | c              | −2607.93                                     | −2230.1                                      |                                                        |                                                          |
| Na <sub>2</sub> S <sub>2</sub> O <sub>4</sub> dithionate          | c              | −1232.2                                      |                                              |                                                        |                                                          |
| std. state                                                        | aq             | −1233.9                                      | −1124.2                                      | 209.2                                                  |                                                          |
| Na <sub>2</sub> S <sub>2</sub> O <sub>7</sub>                     | c              | −1925.1                                      | −1722.1                                      | 202.1                                                  |                                                          |
| Na <sub>2</sub> S <sub>2</sub> O <sub>8</sub>                     | aq             | −1825.1                                      | −1638.9                                      | 362.3                                                  |                                                          |
| Na <sub>2</sub> Te                                                | c              | −349.4                                       |                                              |                                                        |                                                          |
| Na <sub>2</sub> TeO <sub>4</sub>                                  | c              | −1270.7                                      |                                              |                                                        |                                                          |
| Na <sub>2</sub> TiO <sub>3</sub>                                  | c              | −1591.2                                      | −1496.2                                      | 121.67                                                 | 125.65                                                   |
| Na <sub>2</sub> UO <sub>4</sub> beta                              | c              | −1893.3                                      | −1777.78                                     | 166.02                                                 | 146.65                                                   |
| Na <sub>3</sub> UO <sub>4</sub>                                   | c              | −2025.1                                      | −1901.2                                      | 198.20                                                 | 173.01                                                   |
| NaVO <sub>3</sub>                                                 | c              | −1145.79                                     | −1064.12                                     | 113.68                                                 | 97.57                                                    |
| std. state                                                        | aq             | −1128.4                                      | −1045.6                                      | 109                                                    |                                                          |
| Na <sub>3</sub> VO <sub>4</sub>                                   | c              | −1757.87                                     | −1637.83                                     | 190.0                                                  | 164.85                                                   |
| Na <sub>2</sub> V <sub>2</sub> O <sub>7</sub>                     | c              | −2918.84                                     | −2712.52                                     | 318.4                                                  | 269.74                                                   |
| Na <sub>2</sub> WO <sub>4</sub>                                   | c              | −1544.7                                      | −1429.8                                      | 160.3                                                  | 139.8                                                    |
| Na <sub>2</sub> [Zn(CN) <sub>4</sub> ]                            | aq             | −138.1                                       | −77.0                                        | 343                                                    |                                                          |
| Strontium                                                         |                |                                              |                                              |                                                        |                                                          |
| Sr                                                                | c              | 0                                            | 0                                            | 55.0                                                   | 26.79                                                    |
| Sr <sup>2+</sup> std. state                                       | aq             | −545.8                                       | −559.44                                      | −32.6                                                  |                                                          |
| Sr(OAc) <sub>2</sub>                                              | c              | −1487.4                                      |                                              |                                                        |                                                          |
| Sr <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>                  | c              | −3317.1                                      | −3080.3                                      | 255                                                    |                                                          |
| SrBr <sub>2</sub>                                                 | c              | −717.6                                       | −697.1                                       | 135.1                                                  | 75.3                                                     |
|                                                                   | aq             | −788.89                                      | −767.39                                      | 132.2                                                  |                                                          |
| SrCl <sub>2</sub>                                                 | c              | −828.9                                       | −781.1                                       | 114.9                                                  | 75.59                                                    |
| std. state                                                        | aq             | −880.10                                      | −821.95                                      | 80.3                                                   |                                                          |
| Sr(ClO <sub>4</sub> ) <sub>2</sub>                                | c              | −762.69                                      |                                              |                                                        |                                                          |
| std. state                                                        | aq             | −804.46                                      | −576.68                                      | 331.4                                                  |                                                          |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                        | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| SrCO <sub>3</sub>                                | c              | -1220.1                                      | -1140.1                                      | 97.1                                                   | 81.42                                                    |
|                                                  | aq             | -1222.9                                      | -1087.3                                      | -89.5                                                  |                                                          |
| SrC <sub>2</sub> O <sub>4</sub>                  | c              | -1370.7                                      |                                              |                                                        |                                                          |
| SrF <sub>2</sub>                                 | c              | -1216.3                                      | -1164                                        | 82.1                                                   | 70.0                                                     |
| Sr formate                                       | c              | -1393.3                                      |                                              |                                                        |                                                          |
| SrHPO <sub>4</sub>                               | c              | -1821.7                                      | -1688.7                                      | 121                                                    |                                                          |
| Sr(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> | c              | -3134.7                                      |                                              |                                                        |                                                          |
| SrI <sub>2</sub>                                 | c              | -558.1                                       | -557.7                                       | 159.1                                                  | 77.95                                                    |
| std. state                                       | aq             | -656.18                                      | -662.62                                      | 190.0                                                  |                                                          |
| Sr(IO <sub>3</sub> ) <sub>2</sub>                | c              | -1019.2                                      | -855.2                                       | 234                                                    |                                                          |
| SrMoO <sub>4</sub>                               | c              | -1561.1                                      |                                              | 128.9                                                  | 117.07                                                   |
| Sr(NO <sub>2</sub> ) <sub>2</sub>                | c              | -762.3                                       |                                              |                                                        |                                                          |
| Sr(NO <sub>3</sub> ) <sub>2</sub>                | c              | -978.22                                      | -780.0                                       | 194.56                                                 | 149.87                                                   |
| std. state                                       | aq             | -960.52                                      | -782.12                                      | 260.2                                                  |                                                          |
| SrO                                              | c              | -592.0                                       | -561.9                                       | 54.4                                                   | 45.0                                                     |
| SrO <sub>2</sub>                                 | c              | -654.4                                       |                                              | 54                                                     | 79.45                                                    |
| Sr(OH) <sub>2</sub>                              | c              | -959                                         | -881                                         | 97                                                     | 74.9                                                     |
| Sr <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>  | c              | -4122.9                                      |                                              |                                                        |                                                          |
| SrS                                              | c              | -472.4                                       | -467                                         | 68.2                                                   | 48.7                                                     |
| SrSe                                             | c              | -385.8                                       |                                              |                                                        |                                                          |
| SrSeO <sub>3</sub>                               | c              | -1047.7                                      |                                              |                                                        |                                                          |
| SrSeO <sub>4</sub>                               | c              | -1142.7                                      |                                              |                                                        |                                                          |
| SrSiO <sub>3</sub>                               | c              | -1633.9                                      | -1549.8                                      | 96.7                                                   | 88.53                                                    |
| Sr <sub>2</sub> SiO <sub>4</sub>                 | c              | -2304.6                                      | -2191.2                                      | 153.1                                                  | 134.26                                                   |
| SrSO <sub>3</sub>                                | c              | -1177.0                                      |                                              |                                                        |                                                          |
| SrSO <sub>4</sub>                                | c              | -1453.1                                      | -1341.0                                      | 117.0                                                  | 107.78                                                   |
|                                                  | aq             | -1455.1                                      | -1304.0                                      | -12.6                                                  |                                                          |
| Sr <sub>2</sub> TiO <sub>4</sub>                 | c              | -2287.4                                      | -2178.6                                      | 159.0                                                  | 143.68                                                   |
| Sulfur                                           |                |                                              |                                              |                                                        |                                                          |
| S rhombic                                        | c              | 0                                            | 0                                            | 32.054(50)                                             | 22.60                                                    |
| monoclinic                                       | c              | 0.360                                        | -0.070                                       | 33.03                                                  | 23.23                                                    |
|                                                  | g              | 277.17(15)                                   |                                              | 167.829(6)                                             |                                                          |
| S <sub>2</sub> <sup>2-</sup>                     | aq             | 33.1                                         | 85.8                                         | -14.6                                                  |                                                          |
| S <sub>2</sub>                                   | g              | 128.60(30)                                   |                                              | 228.167(10)                                            |                                                          |
| S <sub>8</sub>                                   | g              | 101.25                                       | 49.16                                        | 430.20                                                 | 156.06                                                   |
| S <sub>2</sub> Br <sub>2</sub>                   | lq             | -13.0                                        |                                              |                                                        |                                                          |
| SCl <sub>2</sub>                                 | lq             | -50.0                                        | -28.5                                        | 184                                                    | 91.0                                                     |
| SClF <sub>5</sub>                                | lq             | -1065.7                                      |                                              |                                                        |                                                          |
| S <sub>2</sub> Cl <sub>2</sub>                   | lq             | -59.4                                        | -39                                          | 224                                                    | 124.3                                                    |
| SCN <sup>-</sup>                                 | aq             | 76.4                                         | 92.7                                         | 144.3                                                  | -40.2                                                    |
| SF <sub>4</sub>                                  | g              | -763.2                                       | -722.0                                       | 299.6                                                  | 77.60                                                    |
| SF <sub>6</sub>                                  | g              | -1220.5                                      | -1116.5                                      | 291.5                                                  | 96.96                                                    |
| S <sub>2</sub> F <sub>10</sub>                   | g              | -2064                                        | -1861                                        | 397                                                    | 176.7                                                    |
| SO                                               | g              | 6.3                                          | -19.9                                        | 222.0                                                  | 30.2                                                     |
| SO <sub>2</sub>                                  | g              | -296.81(20)                                  | -300.13                                      | 248.223(50)                                            | 39.88                                                    |
| SO <sub>3</sub>                                  | g              | -395.7                                       | -371.02                                      | 256.77                                                 | 50.66                                                    |
| SOCl <sub>2</sub>                                | g              | -212.50                                      | -198.3                                       | 309.8                                                  | 66.5                                                     |
| SOF <sub>2</sub>                                 | g              | -544                                         | -502                                         | 278.7                                                  | 56.81                                                    |
| SO <sub>2</sub> Cl <sub>2</sub>                  | g              | -364.0                                       | -320.0                                       | 311.9                                                  | 77.01                                                    |
| SO <sub>2</sub> ClF                              | g              | -556                                         | -513                                         | 303                                                    | 71.6                                                     |
| SO <sub>2</sub> F <sub>2</sub>                   | g              | -759                                         | -712                                         | 284.0                                                  | 66.0                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                               | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|-----------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| $\text{SO}_3^{2-}$                      | aq             | − 635.5                                                 | − 486.5                                                 | − 29.0                                                              |                                                                       |
| $\text{SO}_4^{2-}$                      | aq             | − 909.34(40)                                            | − 744.5                                                 | 18.50(40)                                                           | − 293.0                                                               |
| $\text{S}_2\text{O}_3^{2-}$             | aq             | − 652.3                                                 | − 522.5                                                 | 67.0                                                                |                                                                       |
| $\text{S}_2\text{O}_4^{2-}$             | aq             | − 753.5                                                 | − 600.3                                                 | 92.0                                                                |                                                                       |
| $\text{S}_2\text{O}_8^{2-}$             | aq             | − 1344.7                                                | − 1114.9                                                | 244.3                                                               |                                                                       |
| Tantalum                                |                |                                                         |                                                         |                                                                     |                                                                       |
| Ta                                      | c              | 0                                                       | 0                                                       | 41.47                                                               | 25.40                                                                 |
| $\text{TaB}_2$                          | c              | − 209.2                                                 |                                                         | 44.4                                                                | 48.12                                                                 |
| $\text{TaBr}_5$                         | c              | − 598.3                                                 |                                                         | 305.4                                                               | 155.73                                                                |
| TaC                                     | c              | − 144.1                                                 | − 142.7                                                 | 42.37                                                               | 36.79                                                                 |
| $\text{Ta}_2\text{C}$                   | c              | − 197.5                                                 |                                                         | 83.7                                                                | 60.96                                                                 |
| $\text{TaCl}_5$                         | c              | − 859.0                                                 | − 746                                                   | 222                                                                 | 148                                                                   |
| $\text{TaF}_5$                          | c              | − 1903.6                                                |                                                         | 195.0                                                               | 130.46                                                                |
| $\text{Ta}_2\text{H}$                   | c              | − 32.6                                                  | − 69.0                                                  | 79.1                                                                | 90.8                                                                  |
| $\text{TaI}_5$                          | c              | − 490                                                   |                                                         | 343                                                                 | 155.6                                                                 |
| TaN                                     | c              | − 251                                                   |                                                         | 50.6                                                                | 42.1                                                                  |
| $\text{TaO}_2$                          | g              | − 201                                                   | − 209                                                   | 280                                                                 | 44.0                                                                  |
| $\text{Ta}_2\text{O}_5$                 | c              | − 2046                                                  | − 1911.0                                                | 143.1                                                               | 135.0                                                                 |
| $\text{TaOCl}_3$                        | g              | − 780.7                                                 |                                                         | 361.5                                                               | 98.53                                                                 |
| Technetium                              |                |                                                         |                                                         |                                                                     |                                                                       |
| Tc                                      | c              | 0                                                       | 0                                                       | 33.47                                                               | 24.27                                                                 |
| $\text{Tc}_2\text{O}_7$                 | c              | − 1113                                                  |                                                         |                                                                     |                                                                       |
| Tellurium                               |                |                                                         |                                                         |                                                                     |                                                                       |
| Te                                      | c              | 0                                                       | 0                                                       | 49.70                                                               | 25.70                                                                 |
| $\text{TeBr}_4$                         | c              | − 190.4                                                 |                                                         |                                                                     |                                                                       |
| $\text{TeCl}_4$                         | c              | − 326.4                                                 |                                                         | 209                                                                 | 138.5                                                                 |
| $\text{TeF}_6$                          | g              | − 1318.0                                                |                                                         | 335.77                                                              | 116.90                                                                |
| $\text{TeO}_2$                          | c              | − 322.6                                                 | − 270.3                                                 | 79.5                                                                | 63.89                                                                 |
| $\text{Te(OH)}_3^-$                     | aq             | − 322.6                                                 | − 496.1                                                 | 111.7                                                               |                                                                       |
| Terbium                                 |                |                                                         |                                                         |                                                                     |                                                                       |
| Tb                                      | c              | 0                                                       | 0                                                       | 73.22                                                               | 28.91                                                                 |
| $\text{Tb}^{3+}$ std. state             | aq             | − 682.8                                                 | − 651.9                                                 | − 226.0                                                             | 17.0                                                                  |
| $\text{TbCl}_3$                         | c              | − 997.1                                                 |                                                         |                                                                     |                                                                       |
| std. state                              | aq             | − 1184.1                                                | − 1045.6                                                | − 59.0                                                              | − 393.0                                                               |
| $\text{TbO}_2$                          | c              | − 971.5                                                 |                                                         |                                                                     |                                                                       |
| $\text{Tb}_2\text{O}_3$                 | c              | − 1865.2                                                |                                                         |                                                                     | 115.9                                                                 |
| $\text{Tb}_2(\text{SO}_4)_3$ std. state | aq             | − 4131.7                                                | − 3597.4                                                |                                                                     |                                                                       |
| Thallium                                |                |                                                         |                                                         |                                                                     |                                                                       |
| Tl                                      | c              | 0                                                       | 0                                                       | 64.18                                                               | 26.32                                                                 |
| $\text{Tl}^+$ std. state                | aq             | 5.36                                                    | − 32.38                                                 | 125.5                                                               |                                                                       |
| $\text{Tl}^{3+}$ std. state             | aq             | 196.6                                                   | 214.6                                                   | − 192.0                                                             |                                                                       |
| $\text{TlBr}$                           | c              | − 173.2                                                 | − 167.36                                                | 120.5                                                               | 50.50                                                                 |
| std. state                              | aq             | − 116.19                                                | − 136.36                                                | 207.9                                                               |                                                                       |
| $\text{TlBr}_3$                         | aq             | − 168.2                                                 | − 97.1                                                  | 54.0                                                                |                                                                       |
| $\text{TlBrO}_3$                        | c              | − 136.4                                                 | − 53.14                                                 | 168.6                                                               |                                                                       |
| std. state                              | aq             | − 78.2                                                  | − 30.5                                                  | 288.7                                                               |                                                                       |
| $\text{TlCl}$                           | c              | − 204.10                                                | − 184.93                                                | 111.30                                                              | 50.92                                                                 |
| std. state                              | aq             | − 161.80                                                | − 163.64                                                | 182.00                                                              |                                                                       |
| $\text{TlCl}_3$                         | c              | − 315.1                                                 |                                                         |                                                                     |                                                                       |
| std. state                              | aq             | − 305.0                                                 | − 179.1                                                 | − 23.0                                                              |                                                                       |
| $\text{TlClO}_3$                        | aq             | − 93.7                                                  | − 35.6                                                  | 287.9                                                               |                                                                       |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                         | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|-----------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Tl <sub>2</sub> CO <sub>3</sub>   | c              | −700                                         | −614.6                                       | 155.2                                                  |                                                          |
| TlF                               | c              | −324.6                                       |                                              | 83.3                                                   | 54.77                                                    |
| std. state                        | aq             | −327.27                                      | −311.21                                      | 111.7                                                  |                                                          |
| TlI                               | c              | −123.9                                       | −125.39                                      | 127.6                                                  | 52.51                                                    |
| std. state                        | aq             | −49.83                                       | −83.97                                       | 236.8                                                  |                                                          |
| TlNO <sub>3</sub>                 | c              | −243.93                                      | −152.46                                      | 160.7                                                  | 99.50                                                    |
|                                   | aq             | −202.0                                       | −143.7                                       | 272.0                                                  |                                                          |
| Tl <sub>2</sub> O                 | c              | −178.7                                       | −147.3                                       | 126                                                    |                                                          |
| TlOH                              | c              | −238.9                                       | −195.8                                       | 88                                                     |                                                          |
| std. state                        | aq             | −224.64                                      | −189.66                                      | 114.6                                                  |                                                          |
| Tl <sub>2</sub> S                 | c              | −97.1                                        | −93.7                                        | 151.0                                                  |                                                          |
| Tl <sub>2</sub> Se                | c              | −59.0                                        | −59.0                                        | 172.0                                                  |                                                          |
| Tl <sub>2</sub> SO <sub>4</sub>   | c              | −931.8                                       | −830.48                                      | 230.5                                                  |                                                          |
| std. state                        | aq             | −898.56                                      | −809.40                                      | 271.1                                                  |                                                          |
| Thorium                           |                |                                              |                                              |                                                        |                                                          |
| Th                                | c              | 0                                            | 0                                            | 51.8(5)                                                | 27.32                                                    |
|                                   | g              | 602.(6)                                      |                                              | 190.17(5)                                              |                                                          |
| Th <sup>4+</sup> std. state       | aq             | −769.0                                       | −705.1                                       | −422.6                                                 |                                                          |
| ThBr <sub>4</sub>                 | c              | −965.3                                       | −927.2                                       | 230                                                    |                                                          |
| ThC <sub>1.94</sub>               | c              | −146                                         | −147.7                                       | 68.49                                                  | 56.69                                                    |
| ThCl <sub>4</sub>                 | c              | −1186.2                                      | −1094.1                                      | 190.4                                                  | 120.3                                                    |
| ThF <sub>3</sub>                  | g              | −1166.1                                      | −1160.6                                      | 339.2                                                  | 73.3                                                     |
| ThF <sub>4</sub>                  | c              | −2097.8                                      | −2003.4                                      | 142.05                                                 | 110.7                                                    |
| undissoc; std. state              | aq             | −2115.0                                      | −1947.2                                      | −105                                                   |                                                          |
| ThH <sub>2</sub>                  | c              | −139.8                                       | −100.0                                       | 50.71                                                  | 36.69                                                    |
| ThI <sub>4</sub>                  | c              | −664.8                                       | −655.2                                       | 255                                                    |                                                          |
| ThN                               | c              | −391.2                                       | −363.6                                       | 56.07                                                  | 45.2                                                     |
| Th <sub>3</sub> N <sub>4</sub>    | c              | −1315.0                                      | −1212.9                                      | 201                                                    | 155.90                                                   |
| Th(NO <sub>3</sub> ) <sub>4</sub> | c              | −1441.4                                      |                                              |                                                        |                                                          |
| ThO <sub>2</sub>                  | c              | −1226.4(35)                                  | −1169.20                                     | 65.23(20)                                              | 61.76                                                    |
| ThOCl <sub>2</sub>                | c              | −1232.2                                      | −1156.0                                      | 123.4                                                  | 91.25                                                    |
| ThOF <sub>2</sub>                 | c              | −1665.2                                      | −1589.5                                      | 105                                                    |                                                          |
| Th(OH) <sup>3+</sup>              | aq             | −1030.1                                      | −920.5                                       | −343.0                                                 |                                                          |
| Th(OH) <sub>2</sub> <sup>2+</sup> | aq             | −1282.4                                      | −1140.9                                      | −218.0                                                 |                                                          |
| Th <sub>3</sub> P <sub>4</sub>    | c              | −1140.2                                      | −1112.9                                      | 221.8                                                  |                                                          |
| ThS <sub>2</sub>                  | c              | −626.3                                       | −620.1                                       | 96.2                                                   |                                                          |
| Th <sub>2</sub> S <sub>3</sub>    | c              | −1083.7                                      | −1077.0                                      | 180                                                    |                                                          |
| Th(SO <sub>4</sub> ) <sub>2</sub> | c              | −2542.6                                      | −2310.4                                      | 159.0                                                  | 173.47                                                   |
| Thullium                          |                |                                              |                                              |                                                        |                                                          |
| Tm                                | c              | 0                                            | 0                                            | 74.01                                                  | 27.03                                                    |
| Tm <sup>3+</sup> std. state       | aq             | −697.9                                       | −661.9                                       | −243.0                                                 | 25.0                                                     |
| TmCl <sub>3</sub>                 | c              | −986.6                                       |                                              |                                                        |                                                          |
| std. state                        | aq             | −1199.1                                      | −1055.6                                      | −75.0                                                  | −385.0                                                   |
| Tm <sub>2</sub> O <sub>3</sub>    | c              | −1888.7                                      | −1794.5                                      | 139.8                                                  | 116.7                                                    |
| Tin                               |                |                                              |                                              |                                                        |                                                          |
| Sn white                          | c              | 0                                            | 0                                            | 51.08(8)                                               | 26.99                                                    |
|                                   | aq             | 301.2(15)                                    |                                              | 168.492(4)                                             |                                                          |
| gray                              | c              | −2.09                                        | 0.13                                         | 44.14                                                  | 25.77                                                    |
| Sn <sup>2+</sup> in aqueous HCl   | aq             | −8.9(10)                                     | −27.2                                        | −16.7(40)                                              |                                                          |
| Sn <sup>4+</sup> in aqueous HCl   | aq             | 30.5                                         | 2.5                                          | −117                                                   |                                                          |
| SnBr <sub>2</sub>                 | c              | −243.5                                       |                                              |                                                        |                                                          |



**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                      | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|--------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| SnBr <sub>4</sub>              | c              | − 377.4                                      | − 350.2                                      | 264.4                                                  | 136.44                                                   |
|                                | g              | − 314.6                                      | − 331.4                                      | 411.9                                                  | 103.4                                                    |
| SnCl <sub>2</sub>              | c              | − 325.1                                      |                                              | 130                                                    | 79.33                                                    |
|                                | std. state     | − 329.7                                      | − 299.6                                      | 172                                                    |                                                          |
| SnCl <sub>4</sub>              | lq             | − 511.3                                      | − 440.2                                      | 258.6                                                  | 165.3                                                    |
|                                | g              | − 471.5                                      | − 432.2                                      | 365.8                                                  | 98.3                                                     |
| SnH <sub>4</sub>               | g              | 162.8                                        | 188.3                                        | 227.7                                                  | 48.95                                                    |
| SnI <sub>2</sub>               | c              | − 143.5                                      |                                              |                                                        |                                                          |
| SnI <sub>4</sub>               | g              |                                              |                                              | 446.1                                                  | 105.4                                                    |
| SnO tetragonal                 | c              | − 280.71(20)                                 | − 251.9                                      | 57.17(30)                                              | 44.31                                                    |
| SnO <sub>2</sub> tetragonal    | c              | − 577.63(20)                                 | − 515.8                                      | 49.04(10)                                              | 52.59                                                    |
| Sn(OH) <sup>+</sup>            | aq             | − 286.2                                      | − 254.8                                      | 50.0                                                   |                                                          |
| Sn(OH) <sub>2</sub>            | c              | − 561.1                                      | − 491.6                                      | 155.0                                                  |                                                          |
| SnS                            | c              | − 100                                        | − 98.3                                       | 77.0                                                   | 49.25                                                    |
| SnS <sub>2</sub>               | c              | − 167.4                                      |                                              | 87.4                                                   | 70.12                                                    |
| Titanium                       |                |                                              |                                              |                                                        |                                                          |
| Ti                             | c              | 0                                            | 0                                            | 30.72(10)                                              | 25.0                                                     |
|                                | g              | 473.(3)                                      |                                              | 180.298(10)                                            |                                                          |
| TiB                            | c              | − 160                                        | − 160                                        | 35                                                     | 29.7                                                     |
| TiB <sub>2</sub>               | c              | − 280                                        | − 275                                        | 28.5                                                   | 44.3                                                     |
| TiBr <sub>2</sub>              | c              | − 402                                        | − 383                                        | 108                                                    | 78.7                                                     |
| TiBr <sub>3</sub>              | c              | − 548.5                                      | − 523.8                                      | 176.6                                                  | 101.7                                                    |
| TiBr <sub>4</sub>              | c              | − 616.7                                      | − 589.5                                      | 243.5                                                  | 131.5                                                    |
| TiC                            | c              | − 184                                        | − 180                                        | 24.2                                                   | 33.81                                                    |
| TiCl <sub>2</sub>              | c              | − 513.8                                      | − 464.4                                      | 87.4                                                   | 69.8                                                     |
| TiCl <sub>3</sub>              | c              | − 720.9                                      | − 653.5                                      | 139.7                                                  | 97.2                                                     |
| TiCl <sub>4</sub>              | lq             | − 804.2                                      | − 737.2                                      | 252.3                                                  | 145.2                                                    |
|                                | g              | − 763.2(30)                                  | − 726.3                                      | 353.2(40)                                              | 95.4                                                     |
| TiF <sub>3</sub>               | c              | − 1435                                       | − 1362                                       | 88                                                     | 92                                                       |
| TiF <sub>4</sub>               | c              | − 1649                                       | − 1559                                       | 133.96                                                 | 114.27                                                   |
| TiH <sub>2</sub>               | c              | − 144                                        | − 105.1                                      | 29.71                                                  | 30.09                                                    |
| TiI <sub>4</sub>               | c              | − 375                                        | − 371.5                                      | 249.4                                                  | 125.6                                                    |
| TiN                            | c              | − 265.8                                      | − 243.8                                      | 52.73                                                  | 37.08                                                    |
| TiO                            | c              | − 519.7                                      | − 495.0                                      | 50.0                                                   | 39.9                                                     |
| TiO <sub>2</sub>               | c              | − 944.0(8)                                   | − 888.8                                      | 50.62(30)                                              | 55.0                                                     |
| Ti <sub>2</sub> O <sub>3</sub> | c              | − 1520.9                                     | − 1434.2                                     | 78.8                                                   | 97.4                                                     |
| Ti <sub>3</sub> O <sub>5</sub> | c              | − 2459.4                                     | − 2317.4                                     | 129.3                                                  | 154.8                                                    |
| Tungsten                       |                |                                              |                                              |                                                        |                                                          |
| W                              | c              | 0                                            | 0                                            | 32.6                                                   | 24.3                                                     |
| WBr <sub>5</sub>               | c              | − 312                                        | − 270                                        | 272                                                    | 155                                                      |
| WBr <sub>6</sub>               | c              | − 348.5                                      | − 290.8                                      | 314                                                    | 181.4                                                    |
| W(CO) <sub>6</sub>             | c              | − 953.5                                      |                                              | 331.8                                                  | 242.5                                                    |
| WCl <sub>4</sub>               | c              | − 443                                        | − 360                                        | 198.3                                                  | 129.7                                                    |
| WCl <sub>5</sub>               | c              | − 515                                        | − 402                                        | 217.6                                                  | 155.6                                                    |
| WCl <sub>6</sub>               | c              | − 602.5                                      | − 456                                        | 238.5                                                  | 175.4                                                    |
| WF <sub>6</sub>                | lq             | − 1747.7                                     | − 1631.4                                     | 251.5                                                  |                                                          |
|                                | g              | − 1721.7                                     | − 1631.4                                     | 341.1                                                  | 119.0                                                    |
| WO <sub>2</sub>                | c              | − 589.9                                      | − 533.86                                     | 50.5                                                   | 56.1                                                     |
| WO <sub>3</sub>                | c              | − 842.9                                      | − 764.1                                      | 75.9                                                   | 73.8                                                     |
| WO <sub>4</sub> <sup>2−</sup>  | aq             | − 1075.7                                     |                                              |                                                        |                                                          |
| WOCl <sub>4</sub>              | c              | − 671                                        | − 549                                        | 173                                                    | 146                                                      |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | Physical State | $\Delta_f H^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_f G^\circ$<br>$\text{kJ} \cdot \text{mol}^{-1}$ | $S^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ | $C_p^\circ$<br>$\text{J} \cdot \text{deg}^{-1} \cdot \text{mol}^{-1}$ |
|-------------------------------------------------|----------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| WOF <sub>4</sub>                                | c              | −1407                                                   | −1298                                                   | 176.0                                                               | 133.6                                                                 |
| WO <sub>2</sub> Cl <sub>2</sub>                 | c              | −780                                                    | −703                                                    | 200.8                                                               | 104.4                                                                 |
| Uranium                                         |                |                                                         |                                                         |                                                                     |                                                                       |
| U                                               | c              | 0                                                       | 0                                                       | 50.20(20)                                                           | 27.66                                                                 |
|                                                 | g              | 533.(8)                                                 |                                                         | 199.79(10)                                                          |                                                                       |
| U <sup>3+</sup>                                 | aq             | −489.1                                                  | −476.2                                                  | −188.0                                                              |                                                                       |
| U <sup>4+</sup>                                 | aq             | −591.2                                                  | −531.9                                                  | −410.0                                                              |                                                                       |
| UB <sub>2</sub>                                 | c              | −161.6                                                  | −159.4                                                  | 55.52                                                               | 55.77                                                                 |
| UBr <sub>3</sub>                                | c              | −699.2                                                  | −673.6                                                  | 192                                                                 | 108.8                                                                 |
| UBr <sub>4</sub>                                | c              | −802.5                                                  | −767.8                                                  | 238.0                                                               | 128.0                                                                 |
| UBr <sub>5</sub>                                | c              | −810.9                                                  | −769.9                                                  | 293                                                                 | 160.7                                                                 |
| UC                                              | c              | −98.3                                                   | −99.2                                                   | 59.20                                                               | 50.12                                                                 |
| UCl <sub>3</sub>                                | c              | −866.5                                                  | −799.1                                                  | 159.0                                                               | 102.5                                                                 |
| UCl <sub>4</sub>                                | c              | −1019.2                                                 | −930.1                                                  | 197.1                                                               | 122.0                                                                 |
|                                                 | aq             | −1259.8                                                 | −1056.8                                                 | −184.0                                                              |                                                                       |
| UCl <sub>5</sub>                                | c              | −1058                                                   | −950                                                    | 242.7                                                               | 144.6                                                                 |
| UCl <sub>6</sub>                                | c              | −1092                                                   | −962                                                    | 285.8                                                               | 175.7                                                                 |
| UF <sub>3</sub>                                 | c              | −1502.1                                                 | −1433.4                                                 | 123.43                                                              | 95.10                                                                 |
| UF <sub>4</sub>                                 | c              | −1921.2                                                 | −1823.3                                                 | 151.67                                                              | 116.02                                                                |
| UF <sub>5</sub>                                 | c              | −2075.3                                                 | −1958.6                                                 | 199.6                                                               | 132.3                                                                 |
| UF <sub>6</sub>                                 | c              | −2197.0                                                 | −2068.6                                                 | 227.6                                                               | 166.8                                                                 |
| UH <sub>3</sub>                                 | c              | −127.2                                                  | −72.8                                                   | 63.68                                                               | 49.29                                                                 |
| UI <sub>3</sub>                                 | c              | −460.7                                                  | −459.8                                                  | 222                                                                 | 112.1                                                                 |
| UI <sub>4</sub>                                 | c              | −512.1                                                  | −506.7                                                  | 264                                                                 | 134.3                                                                 |
| UN                                              | c              | −290.8                                                  | −265.7                                                  | 62.43                                                               | 47.57                                                                 |
| UO <sub>2</sub>                                 | c              | −1085.0(10)                                             | −1031.8                                                 | 77.03(20)                                                           | 63.60                                                                 |
| UO <sub>2</sub> <sup>2+</sup> std. state        | aq             | −1019.0(15)                                             | −953.5                                                  | −98.2(30)                                                           |                                                                       |
| UO <sub>3</sub> gamma                           | c              | −1223.8(12)                                             | −1145.7                                                 | 96.11(40)                                                           | 81.67                                                                 |
| U <sub>3</sub> O <sub>7</sub>                   | c              | −3427.1                                                 | −3242.9                                                 | 250.5                                                               | 215.5                                                                 |
| U <sub>3</sub> O <sub>8</sub>                   | c              | −3574.8(25)                                             | −3369.8                                                 | 282.55(50)                                                          | 238.36                                                                |
| U <sub>4</sub> O <sub>9</sub>                   | c              | −4510.4                                                 | −4275.1                                                 | 334.1                                                               | 293.3                                                                 |
| UOBr <sub>2</sub>                               | c              | −973.6                                                  | −929.7                                                  | 158.00                                                              | 98.00                                                                 |
| UOCl <sub>2</sub>                               | c              | −1066.9                                                 | −996.2                                                  | 138.32                                                              | 95.06                                                                 |
| UOF <sub>2</sub>                                | c              | −1499.1                                                 | −1428.8                                                 | 119.2                                                               |                                                                       |
| UO <sub>2</sub> (OAc) <sub>2</sub>              | c              | −1963.55                                                |                                                         |                                                                     |                                                                       |
| UO <sub>2</sub> Br <sub>2</sub>                 | c              | −1137.6                                                 | −1066.5                                                 | 169.5                                                               |                                                                       |
| UO <sub>2</sub> Cl <sub>2</sub>                 | c              | −1243.9                                                 | −1146.4                                                 | 150.5                                                               | 107.86                                                                |
| std. state                                      | aq             | −1353.9                                                 | −1215.9                                                 | 15.5                                                                |                                                                       |
| UO <sub>2</sub> CO <sub>3</sub>                 | c              | −1691.2                                                 | −1562.7                                                 | 138                                                                 |                                                                       |
| std. state                                      | aq             | −1696.6                                                 | −1481.6                                                 | −154.4                                                              |                                                                       |
| UO <sub>2</sub> C <sub>2</sub> O <sub>4</sub>   | c              | −1796.94                                                |                                                         |                                                                     |                                                                       |
| UO <sub>2</sub> F <sub>2</sub>                  | c              | −1653.5                                                 | −1557.4                                                 | 135.56                                                              | 103.22                                                                |
| std. state                                      | aq             | −1684.0                                                 | −1551.3                                                 | −125.1                                                              |                                                                       |
| UO <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> | c              | −1349.3                                                 | −1105.0                                                 | 243                                                                 |                                                                       |
| std. state                                      | aq             | −1434.3                                                 | −1176.1                                                 | 195.4                                                               |                                                                       |
| UO <sub>2</sub> (OH) <sub>2</sub> std. state    | aq             | −1479.5                                                 | −1267.8                                                 | −118.8                                                              |                                                                       |
| UO <sub>2</sub> SO <sub>4</sub>                 | c              | −1845.1                                                 | −1683.6                                                 | 154.8                                                               | 145.2                                                                 |
| std. state                                      | aq             | −1928.8                                                 | −1698.3                                                 | −77.4                                                               |                                                                       |
| US <sub>2</sub>                                 | c              | −527                                                    | −526.4                                                  | 110.42                                                              | 74.64                                                                 |
| US <sub>3</sub>                                 | c              | −549.4                                                  | −547.3                                                  | 138.49                                                              | 95.60                                                                 |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                    | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Vanadium                                     |                |                                              |                                              |                                                        |                                                          |
| V                                            | c              | 0                                            | 0                                            | 28.94                                                  | 24.90                                                    |
| VBr <sub>4</sub>                             | g              | -336.8                                       |                                              |                                                        |                                                          |
| VCl <sub>2</sub>                             | c              | -452                                         | -406                                         | 97.1                                                   | 72.22                                                    |
| VCl <sub>3</sub>                             | c              | -580.7                                       | -511.3                                       | 131.0                                                  | 93.18                                                    |
| VCl <sub>4</sub>                             | lq             | -569.4                                       | -503.8                                       | 255.0                                                  | 161.7                                                    |
| VF <sub>5</sub>                              | lq             | -1480.3                                      | -1373.2                                      | 175.7                                                  |                                                          |
|                                              | g              | -1433.9                                      | -1369.8                                      | 320.9                                                  | 98.58                                                    |
| VN                                           | c              | -217.15                                      | -191.08                                      | 37.28                                                  | 38.00                                                    |
| VO                                           | c              | -431.8                                       | -404.2                                       | 39.0                                                   | 45.5                                                     |
| VO <sub>2</sub>                              | c              | -717.6                                       |                                              | 51.5                                                   | 62.59                                                    |
| VO <sub>2</sub> <sup>+</sup> std. state      | aq             | -649.8                                       | -587.0                                       | -42.3                                                  |                                                          |
| VO <sub>3</sub> <sup>3+</sup> std. state     | aq             | -486.6                                       | -446.4                                       | -133.9                                                 |                                                          |
| VO <sub>3</sub> <sup>-</sup> std. state      | aq             | -888.3                                       | -783.7                                       | 50.2                                                   |                                                          |
| V <sub>2</sub> O <sub>3</sub>                | c              | -1218.8                                      | -1139.3                                      | 98.3                                                   | 103.2                                                    |
| V <sub>2</sub> O <sub>4</sub>                | c              | -1427                                        | -1318.4                                      | 103                                                    | 115.4                                                    |
| V <sub>2</sub> O <sub>5</sub>                | c              | -1550                                        | -1419.3                                      | 130                                                    | 130.6                                                    |
| V <sub>3</sub> O <sub>5</sub>                | c              | -1933                                        | -1803                                        | 163                                                    |                                                          |
| VOCl <sub>3</sub>                            | lq             | -734.7                                       | -668.6                                       | 244.4                                                  | 150.62                                                   |
|                                              | g              | -695.6                                       | -659.3                                       | 344.4                                                  | 89.9                                                     |
| VOSO <sub>4</sub>                            | c              | -1309.2                                      | -1169.9                                      | 108.8                                                  |                                                          |
| Xenon                                        |                |                                              |                                              |                                                        |                                                          |
| Xe                                           | g              | 0                                            | 0                                            | 169.685(3)                                             | 20.786                                                   |
| XeF <sub>2</sub>                             | c              | -164.0                                       |                                              |                                                        |                                                          |
| XeF <sub>4</sub>                             | c              | -261.5                                       | -123.0                                       |                                                        |                                                          |
| XeF <sub>6</sub>                             | c              | -360                                         |                                              |                                                        |                                                          |
|                                              | g              | -297                                         |                                              |                                                        |                                                          |
| XeO <sub>3</sub>                             | c              | 402                                          |                                              |                                                        |                                                          |
| XeOF <sub>4</sub>                            | lq             | 146                                          |                                              |                                                        |                                                          |
| Ytterbium                                    |                |                                              |                                              |                                                        |                                                          |
| Yb                                           | c              | 0                                            | 0                                            | 59.87                                                  | 26.74                                                    |
| Yb <sup>2+</sup> std. state                  | aq             |                                              | -527.0                                       |                                                        |                                                          |
| Yb <sup>3+</sup> std. state                  | aq             | -674.5                                       | -643.9                                       | 238.0                                                  | 25.0                                                     |
| Yb(OAc) <sub>3</sub> undissoc; std. state    | aq             | -2105.0                                      | -1772.84                                     | 183.3                                                  |                                                          |
| YbCl <sub>2</sub>                            | c              | -799.6                                       |                                              |                                                        |                                                          |
| YbCl <sub>3</sub>                            | c              | -959.8                                       |                                              |                                                        |                                                          |
| std. state                                   | aq             | -1176.1                                      | -1037.6                                      | -71.0                                                  | -385.0                                                   |
| Yb(NO <sub>3</sub> ) <sub>3</sub> std. state | aq             | -1296.6                                      |                                              |                                                        |                                                          |
| Yb <sub>2</sub> O <sub>3</sub>               | c              | -1814.6                                      | -1726.7                                      | 133.1                                                  | 115.35                                                   |
| Yttrium                                      |                |                                              |                                              |                                                        |                                                          |
| Y                                            | c              | 0                                            | 0                                            | 44.4                                                   | 26.51                                                    |
| Y <sup>3+</sup> std. state                   | aq             | -723.4                                       | -693.7                                       | -251.0                                                 |                                                          |
| YCl <sub>3</sub>                             | c              | -1000                                        |                                              | 136.8                                                  | 75.0                                                     |
| YF <sub>3</sub>                              | c              | -1718.8                                      | -1644.7                                      | 100                                                    |                                                          |
| Y <sub>2</sub> O <sub>3</sub>                | c              | -1905.31                                     | -1816.65                                     | 99.08                                                  | 102.51                                                   |
| Y(OH) <sub>3</sub>                           | c              | -1435                                        | -1291                                        | 99.2                                                   |                                                          |
| Zinc                                         |                |                                              |                                              |                                                        |                                                          |
| Zn                                           | c              | 0                                            | 0                                            | 41.63(15)                                              | 25.40                                                    |
|                                              | g              | 130.40(40)                                   |                                              | 160.990(4)                                             |                                                          |
| Zn <sup>2+</sup> std. state                  | aq             | -153.39(20)                                  | -147.1                                       | -109.8(5)                                              | 46.0                                                     |

**TABLE 6.3** Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of the Elements and Inorganic Compounds (*Continued*)

| Substance                                    | Physical State | $\Delta_f H^\circ$<br>kJ · mol <sup>-1</sup> | $\Delta_f G^\circ$<br>kJ · mol <sup>-1</sup> | $S^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> | $C_p^\circ$<br>J · deg <sup>-1</sup> · mol <sup>-1</sup> |
|----------------------------------------------|----------------|----------------------------------------------|----------------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| ZnBr <sub>2</sub>                            | c              | -328.65                                      | -312.13                                      | 138.5                                                  | 65.7                                                     |
| std. state                                   | aq             | -396.98                                      | -354.97                                      | 52.72                                                  | -238.0                                                   |
| ZnCl <sub>2</sub>                            | c              | -415.05                                      | -369.45                                      | 111.46                                                 | 71.34                                                    |
| std. state                                   | aq             | -488.19                                      | -409.53                                      | 0.84                                                   | -226.0                                                   |
| Zn(CN) <sub>4</sub> <sup>2-</sup> std. state | aq             | 342.3                                        | 446.9                                        | 226                                                    |                                                          |
| ZnCO <sub>3</sub>                            | c              | -812.78                                      | -731.57                                      | 82.4                                                   | 79.71                                                    |
| ZnF <sub>2</sub>                             | c              | -764.4                                       | -713.3                                       | 73.68                                                  | 65.7                                                     |
| std. state                                   | aq             | -819.14                                      | -704.67                                      | -139.8                                                 | -167.0                                                   |
| ZnI <sub>2</sub>                             | c              | -208.03                                      | -208.95                                      | 161.1                                                  | 65.69                                                    |
|                                              | aq             | -264.3                                       | -250.2                                       | 110.5                                                  | -238.0                                                   |
| Zn(NO <sub>3</sub> ) <sub>2</sub>            | c              | -483.7                                       |                                              |                                                        |                                                          |
|                                              | aq             | -568.6                                       | -369.6                                       | 180.7                                                  | -126.0                                                   |
| ZnO                                          | c              | -350.46(27)                                  | -320.52                                      | 43.65(40)                                              | 40.25                                                    |
| Zn(OH) <sub>2</sub>                          | c              | -641.91                                      | -553.59                                      | 81.2                                                   |                                                          |
| std. state                                   | aq             | -613.88                                      | -461.62                                      | -133.5                                                 | -251                                                     |
| ZnS sphalerite                               | c              | -205.98                                      | -201.29                                      | 57.7                                                   | 46.02                                                    |
| wurtzite                                     | c              | -192.6                                       |                                              |                                                        |                                                          |
| ZnSe                                         | c              | -163                                         | -163                                         | 84.0                                                   |                                                          |
| ZnSO <sub>4</sub>                            | c              | -982.84                                      | -871.5                                       | 110.5                                                  | 99.2                                                     |
|                                              | aq             | -1063.2                                      | -891.6                                       | -92.0                                                  | -247.0                                                   |
| Zn <sub>2</sub> SiO <sub>4</sub>             | c              | -1636.7                                      | -1523.2                                      | 131.42                                                 | 123.3                                                    |
| <b>Zirconium</b>                             |                |                                              |                                              |                                                        |                                                          |
| Zr                                           | c              | 0                                            | 0                                            | 39.0                                                   | 25.40                                                    |
| ZrB                                          | c              | -322                                         | -318.2                                       | 35.94                                                  | 48.24                                                    |
| ZrBr <sub>2</sub>                            | c              | -405                                         | -382                                         | 116                                                    | 86.7                                                     |
| ZrBr <sub>4</sub>                            | c              | -760.7                                       | -725.3                                       | 224                                                    | 124.8                                                    |
| ZrC                                          | c              | 197                                          | -193                                         | 33.32                                                  | 37.90                                                    |
| ZrCl <sub>2</sub>                            | c              | -502.0                                       | -386                                         | 110                                                    | 72.6                                                     |
| ZrCl <sub>3</sub>                            | c              | -714                                         | -646                                         | 146                                                    | 96                                                       |
| ZrCl <sub>4</sub>                            | c              | -981                                         | -890                                         | 181.4                                                  | 119.8                                                    |
| ZrF <sub>2</sub>                             | c              | -962                                         | -913                                         | 75                                                     | 66                                                       |
| ZrF <sub>4</sub>                             | c              | -1911.3                                      | -1810.0                                      | 104.7                                                  | 103.6                                                    |
| ZnH <sub>2</sub>                             | c              | -169.0                                       | -128.8                                       | 35.0                                                   | 31.0                                                     |
| ZrI <sub>2</sub>                             | c              | -259                                         | -258                                         | 150.2                                                  | 94.1                                                     |
| ZrI <sub>3</sub>                             | c              | -397.5                                       | -394.9                                       | 204.6                                                  | 103.8                                                    |
| ZrI <sub>4</sub>                             | c              | -488                                         | -485.4                                       | 260                                                    | 127.8                                                    |
| ZrN                                          | c              | -365                                         | -336.7                                       | 38.86                                                  | 40.44                                                    |
| ZrO <sub>2</sub>                             | c              | -1100.6                                      | -1042.8                                      | 50.36                                                  | 56.19                                                    |
| ZrSiO <sub>4</sub>                           | c              | -2033.4                                      | -1919.1                                      | 84.1                                                   | 98.7                                                     |
| ZrSO <sub>4</sub>                            | c              | -2217.1                                      |                                              |                                                        | 172.0                                                    |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds

*Abbreviations Used in the Table*

$\Delta Hm$ , enthalpy of melting (at the melting point) in  $\text{kJ} \cdot \text{mol}^{-1}$   
 $\Delta Hv$ , enthalpy of vaporization (at the boiling point) in  $\text{kJ} \cdot \text{mol}^{-1}$   
 $\Delta Hs$ , enthalpy of sublimation (or vaporization at 298 K) in  $\text{kJ} \cdot \text{mol}^{-1}$   
 $C_p$ , specific heat (at temperature specified on the Kelvin scale) for the physical state in existence (or specified: c, lq, g) at that temperature in  $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   
 $\Delta Ht$ , enthalpy of transition (at temperature specified, superscript, measured in degrees Celsius) in  $\text{kJ} \cdot \text{mol}^{-1}$

| Substance                                                | $\Delta Hm$ | $\Delta Hv$ | $\Delta Hs$          | $C_p$     |           |         |          |
|----------------------------------------------------------|-------------|-------------|----------------------|-----------|-----------|---------|----------|
|                                                          |             |             |                      | 400 K     | 600 K     | 800 K   | 1000 K   |
| Aluminum                                                 |             |             |                      |           |           |         |          |
| Al                                                       | 10.71       | 294.0       | 326.4                | 25.8      | 27.9      | 30.6    | 34.9(lq) |
| Al(BH <sub>4</sub> ) <sub>3</sub>                        |             | 30          |                      |           |           |         |          |
| Al <sub>6</sub> BeO <sub>10</sub>                        | 402         |             |                      | 324.3     | 380.6     | 407.8   | 425.2    |
| AlBr <sub>3</sub>                                        | 11.25       | 23.5        |                      | 125.0     | 125.0     | 125.0   | 125.0    |
| Al <sub>4</sub> C <sub>3</sub>                           |             |             |                      | 138.5     | 159.2     | 169.7   | 176.1    |
| AlCl <sub>3</sub>                                        | 35.4        |             | 116                  | 100.1     | 117.7     | 135.2   | 152.8    |
| AlF <sub>3</sub> , $\Delta Ht = 0.56^{455}$              | 98          |             |                      | 86.3      | 97.3      | 98.5    | 100.8    |
| AlI <sub>3</sub>                                         | 15.9        | 32.2        | 112                  | 108.5     | 121.3     |         |          |
| AlN                                                      |             |             |                      | 36.7      | 43.5      | 46.8    | 48.5     |
| Al <sub>2</sub> O <sub>3</sub> corundum                  | 111.4       |             |                      | 96.1      | 112.5     | 120.1   | 124.8    |
| AlOCl                                                    |             |             |                      | 64.3      | 72.6      | 76.9    | 79.3     |
| Al <sub>2</sub> SiO <sub>5</sub> andalusite              |             |             |                      | 149.6     | 174.5     | 186.1   | 194.0    |
| kyanite                                                  |             |             |                      | 148.3     | 176.2     | 188.3   | 196.2    |
| sillimanite                                              |             |             |                      | 147.5     | 173.0     | 185.0   | 193.5    |
| Al <sub>6</sub> Si <sub>2</sub> O <sub>13</sub> mullite  |             |             |                      | 390.7     | 459.8     | 494.1   | 513.4    |
| Al <sub>2</sub> S <sub>3</sub>                           | 55          |             |                      | 115.0     | 124.1     | 129.7   | 134.0    |
| Al <sub>2</sub> TiO <sub>5</sub>                         |             |             |                      | 162.0     | 182.8     | 192.9   | 200.0    |
| Americium                                                |             |             |                      |           |           |         |          |
| Am                                                       | 14.39       |             |                      |           |           |         |          |
| Ammonium                                                 |             |             |                      |           |           |         |          |
| NH <sub>3</sub>                                          | 5.66        | 23.35       | 19.86                | 38.7      | 45.3      | 51.1    | 56.2     |
| ND <sub>3</sub> ammonia- <i>d</i> <sub>3</sub>           |             |             |                      | 42.9      | 51.5      | 58.6    | 64.3     |
| NH <sub>4</sub> Br, $\Delta Ht = 3.22^{138}$             |             |             |                      |           |           |         |          |
| NH <sub>4</sub> Cl, $\Delta Ht = 1.046^{-30.6}$          |             |             |                      | 103       |           |         |          |
| $\Delta Ht = 3.950^{184.6}$                              |             |             |                      |           |           |         |          |
| NH <sub>4</sub> ClO <sub>4</sub>                         |             |             |                      | 148.7     |           |         |          |
| NH <sub>4</sub> I, $\Delta Ht = 2.93^{-13}$              | 20.9        |             | 168.5 <sup>525</sup> | 89.0      | 103.3     | 117.7   |          |
| NH <sub>4</sub> NO <sub>3</sub>                          | 6.40        |             |                      |           |           |         |          |
| Antimony                                                 |             |             |                      |           |           |         |          |
| Sb                                                       | 19.87       | 193.43      |                      | 25.9      | 27.7      | 29.5    | 31.4     |
| SbBr <sub>3</sub>                                        | 14.6        | 59          |                      | 125.5(lq) | 81.6(g)   | 82.2    | 82.5     |
| SbCl <sub>3</sub>                                        | 12.7        | 45.2        |                      | 123.4(lq) | 81.6(g)   | 82.2    | 82.5     |
| SbCl <sub>5</sub>                                        | 10.0        | 48.4        |                      |           |           |         |          |
| SbH <sub>3</sub>                                         |             | 21.3        |                      |           |           |         |          |
| SbI <sub>3</sub>                                         | 22.8        | 68.6        |                      | 106.6(lq) | 143.5(lq) | 82.2(g) | 82.5(g)  |
| Sb <sub>2</sub> O <sub>3</sub> , $\Delta Ht = 7.1^{573}$ | 54.4        | 74.6        |                      | 108.5     | 122.8     | 137.1   | 150.6    |
| Sb <sub>2</sub> S <sub>3</sub>                           |             |             |                      | 123.3     | 134.4     | 145.4   |          |
| Argon                                                    |             |             |                      |           |           |         |          |
| Ar                                                       | 1.12        | 6.43        |                      | 20.8      | 20.8      | 20.8    | 20.8     |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                  | $\Delta Hm$ | $\Delta Hv$ | $\Delta Hs$ | $C_p$     |          |           |           |
|----------------------------------------------------------------------------|-------------|-------------|-------------|-----------|----------|-----------|-----------|
|                                                                            |             |             |             | 400 K     | 600 K    | 800 K     | 1000 K    |
| Arsenic                                                                    |             |             |             |           |          |           |           |
| As                                                                         | 24.44       |             |             | 25.6      | 27.5     | 29.3      |           |
| AsBr <sub>3</sub>                                                          | 11.7        | 41.8        |             |           |          |           |           |
| AsCl <sub>3</sub>                                                          | 10.1        | 35.0        |             | 133.5(lq) | 88.3(g)  | 88.3      |           |
| AsF <sub>3</sub>                                                           | 10.4        | 29.7        |             |           |          |           |           |
| AsF <sub>5</sub>                                                           |             | 20.8        |             |           |          |           |           |
| AsH <sub>3</sub>                                                           |             | 16.7        |             | 45.4      | 53.2     | 58.8      | 63.9      |
| AsI <sub>3</sub>                                                           |             | 59.3        |             |           |          |           |           |
| As <sub>2</sub> O <sub>3</sub>                                             | 18.4        |             |             | 116.4     |          |           |           |
| Barium                                                                     |             |             |             |           |          |           |           |
| Ba                                                                         | 7.12        | 140.3       |             | 33.2      | 33.9(c)  |           | 39.1(lq)  |
| BaBr <sub>2</sub>                                                          | 32.2        |             |             | 79.2      | 83.5     | 87.9      | 92.2      |
| BaCl <sub>2</sub> , $\Delta Ht = 16.9^{925}$                               | 15.85       | 246.4       |             | 77.3      | 80.4     | 84.3      | 89.5      |
| BaCO <sub>3</sub> , $\Delta Ht = 18.8^{806}$                               | 40          |             |             | 99.0      | 113.0    | 124.2     | 134.6     |
| BaF <sub>2</sub> , $\Delta Ht = 2.67^{1207}$                               | 17.8        | 285.4       | 405.1       | 75.9      | 80.3     | 84.9      | 94.6      |
| BaH <sub>2</sub>                                                           | 25          |             |             |           |          |           |           |
| BaI <sub>2</sub>                                                           | 26.5        | 43.9        | 302.5       | 79.5      | 83.5     | 87.5(c)   | 113.0(lq) |
| BaMoO <sub>4</sub>                                                         |             |             |             | 129.5     | 143.5    | 152.2     | 159.3     |
| BaO                                                                        | 46          | 330.6       | 424.3       | 49.9      | 53.2     | 55.4      | 57.1      |
| Ba(OH) <sub>2</sub>                                                        | 16          |             |             | 112.6     | 122.7(c) | 141.0(lq) |           |
| BaS                                                                        | 63          |             |             |           |          |           |           |
| BaSO <sub>4</sub>                                                          | 40          |             |             | 119.4     | 131.6    | 135.9     | 137.9     |
| BaTiO <sub>3</sub> , $\Delta Ht = 0.067^{75}$                              |             |             |             | 111.5     | 121.8    | 126.1     | 128.7     |
| Beryllium                                                                  |             |             |             |           |          |           |           |
| Be                                                                         | 7.895       | 297         | 291         | 20.0      | 23.3     | 25.5      | 27.3      |
| BeAl <sub>2</sub> O <sub>4</sub> , chrysoberyl                             | 170.0       |             |             | 130.3     | 155.0    | 166.8     | 174.2     |
| BeBr <sub>2</sub>                                                          | 18          | 100.0       | 515         | 70.6      | 77.6(c)  | 113.0(lq) | 113.0     |
| Be <sub>2</sub> C                                                          | 75.3        |             |             | 47.6      | 51.9     | 64.7      | 73.2      |
| BeCl <sub>2</sub> , $\Delta Ht = 6.8^{403}$                                | 8.66        | 105         | 136.0       | 68.7      | 75.8(c)  | 121.4(lq) | 121.4     |
| BeF <sub>2</sub> , $\Delta Ht = 0.92^{227}$                                | 4.77        | 199.4       |             | 62.5      | 67.5     | 74.1(c)   | 85.6(lq)  |
| BeI <sub>2</sub>                                                           | 18          | 70.5        | 125         | 76.9      | 84.2     |           |           |
| Be <sub>3</sub> N <sub>2</sub>                                             | 129.3       |             |             | 84.4      | 106.5    | 117.6     | 123.6     |
| BeO, $\Delta Ht = 6.7^{2100}$                                              | 86          |             |             | 33.8      | 42.4     | 46.7      | 49.3      |
| BeS                                                                        |             |             |             | 120.8     | 149.2    | 166.0     | 174.1     |
| Be <sub>2</sub> SiO <sub>4</sub>                                           |             |             |             | 103.9     | 126.8    | 149.8     | 174.4     |
| BeSO <sub>4</sub> , $\Delta Ht = 1.113^{590}$<br>$\Delta Ht = 19.55^{635}$ | 6           |             |             | 103.9     | 126.8    | 149.8     | 174.4     |
| BeWO <sub>4</sub>                                                          |             |             |             | 113.0     | 131.3    | 142.9     | 153.0     |
| Bismuth                                                                    |             |             |             |           |          |           |           |
| Bi                                                                         | 11.30       | 151         |             | 27.0(c)   | 31.8(lq) | 31.8      | 31.8      |
| BiBr <sub>3</sub>                                                          | 21.7        | 75.4        |             |           |          |           |           |
| BiCl <sub>3</sub>                                                          | 10.9        | 72.6        |             |           |          |           |           |
| BiI <sub>3</sub>                                                           |             | 20.9        |             |           |          |           |           |
| Bi <sub>2</sub> O <sub>3</sub> , $\Delta Ht = 116.7^{717}$                 | 28.5        |             |             | 116.9     | 123.6    | 130.3     | 137.0     |
| Bi <sub>2</sub> S <sub>3</sub>                                             |             |             |             | 131.1     | 136.2    | 141.3     | 146.4     |
| Bi <sub>2</sub> Te <sub>3</sub>                                            | 120.5       |             |             | 164.3     | 179.7    | 192.3     |           |
| Boron                                                                      |             |             |             |           |          |           |           |
| B                                                                          | 50.2        | 480         | 552         | 15.7      | 20.8     | 23.4      | 25.0      |
| BBr <sub>3</sub>                                                           |             | 30.5        |             | 72.6(g)   | 77.6     | 79.8      | 81.1      |
| B <sub>4</sub> C                                                           | 105         |             |             | 76.4      | 98.4     | 107.7     | 114.3     |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$     |          |           |        |
|------------------------------------------------------------------------------|--------------|--------------|--------------|-----------|----------|-----------|--------|
|                                                                              |              |              |              | 400 K     | 600 K    | 800 K     | 1000 K |
| BCl <sub>3</sub>                                                             | 2.10         | 23.8         | 23.1         | 68.4(g)   | 75.0     | 78.2      | 79.8   |
| BF <sub>3</sub>                                                              | 4.20         | 19.3         | 57.5         | 67.1      | 72.6     | 75.8      |        |
| F <sub>2</sub> B-BF <sub>2</sub>                                             |              | 28           |              |           |          |           |        |
| BH <sub>3</sub>                                                              |              |              |              | 38.9      | 45.4     | 52.3      | 58.4   |
| B <sub>2</sub> H <sub>6</sub>                                                | 4.44         | 14.3         |              | 74.3      | 101.3    | 121.7     | 136.4  |
| B <sub>4</sub> H <sub>9</sub>                                                | 6.13         | 28.4         |              | 130.2(g)  | 187.6    | 227.4     | 254.4  |
| B <sub>4</sub> H <sub>10</sub>                                               |              | 27.1         |              |           |          |           |        |
| B <sub>5</sub> H <sub>11</sub>                                               |              | 31.8         |              |           |          |           |        |
| B <sub>10</sub> H <sub>14</sub>                                              | 32.5         | 48.5         | 76.7         | 250.0(lq) | 351.6(g) | 417.2     | 460.4  |
| BI <sub>3</sub>                                                              |              | 40.5         |              |           |          |           |        |
| BN                                                                           | 81           |              | 728          | 26.3      | 35.2     | 40.5      | 44.3   |
| B <sub>3</sub> N <sub>3</sub> H <sub>6</sub> borazine                        |              | 32.1         |              | 126.9     | 169.4    | 197.2     | 216.6  |
| B <sub>2</sub> O <sub>3</sub>                                                | 24.56        | 390.4        |              | 77.9      | 98.1(c)  | 129.7(lq) | 129.7  |
| B <sub>3</sub> O <sub>3</sub> H <sub>3</sub> boroxin                         |              |              | 44.8         | 120.1     | 162.8    | 194.6     | 214.2  |
| Bromine                                                                      |              |              |              |           |          |           |        |
| Br <sub>2</sub>                                                              | 10.57        | 29.96        | 30.9         | 36.7(g)   | 37.3     | 37.6      | 37.8   |
| BrCl                                                                         | 10.4         | 34.7         |              |           |          |           |        |
| BrF                                                                          |              | 25.1         |              |           |          |           |        |
| BrF <sub>3</sub>                                                             | 12.05        | 47.6         |              | 72.6      | 78.0     | 80.1      | 81.2   |
| BrF <sub>5</sub>                                                             | 5.67         | 30.6         |              | 113.0     | 123.2    | 127.3     | 129.3  |
| Cadmium                                                                      |              |              |              |           |          |           |        |
| Cd                                                                           | 6.19         | 99.9         |              | 27.1(c)   | 29.7(lq) | 29.7      | 29.7   |
| CdBr <sub>2</sub>                                                            | 20.9         | 115          |              |           |          |           |        |
| CdCl <sub>2</sub>                                                            | 48.58        | 124.3        |              | 79.8      | 86.3     | 92.7      | 104.6  |
| CdF <sub>2</sub>                                                             | 22.6         | 214          |              |           |          |           |        |
| CdI <sub>2</sub>                                                             | 15.3         | 115          |              |           |          |           |        |
| Cd(NO <sub>3</sub> ) <sub>2</sub> · 4H <sub>2</sub> O                        | 32.6         |              |              |           |          |           |        |
| CdO                                                                          |              |              | 225.1        | 43.8      | 45.6     | 47.3      | 49.1   |
| CdS                                                                          |              |              | 209.6        | 55.5      | 56.2     | 57.0      | 57.7   |
| CdSO <sub>4</sub>                                                            |              |              |              | 108.3     | 123.8    | 139.2     | 154.7  |
| Calcium                                                                      |              |              |              |           |          |           |        |
| Ca, $\Delta H_t = 0.93^4$                                                    | 8.54         | 154.7        |              | 26.9      | 30.0     | 33.8      | 39.7   |
| Ca(BO <sub>2</sub> ) <sub>2</sub>                                            | 74.1         |              |              | 125.0     | 144.9    | 157.2     | 176.2  |
| CaB <sub>4</sub> O <sub>7</sub>                                              | 113.4        |              |              | 202.0     | 243.0    | 267.7     | 287.8  |
| CaBr <sub>2</sub>                                                            | 29.1         | 200          | 298.3        | 78.0      | 80.5     | 83.5      | 88.6   |
| CaC <sub>2</sub> carbide                                                     | 32           |              |              |           |          |           |        |
| CaCl <sub>2</sub>                                                            | 28.05        | 235          |              | 75.6      | 78.2     | 80.9      | 85.8   |
| CaCN <sub>2</sub> cyanamide                                                  | 0.432        |              |              |           |          |           |        |
| CaCO <sub>3</sub>                                                            | 36           |              |              |           |          |           |        |
| CaF <sub>2</sub> , $\Delta H_t = 4.8^{1151}$                                 | 29.3         | 308.9        | 441          | 73.9      | 78.5     | 83.9      | 90.1   |
| CaH <sub>2</sub>                                                             | 6.7          |              |              |           |          |           |        |
| CaI <sub>2</sub>                                                             | 41.8         | 179.4        | 243          | 79.2      | 83.1     | 87.1      | 91.0   |
| Ca[Mg(CO <sub>3</sub> ) <sub>2</sub> ] dolomite                              |              |              |              | 143.3     | 163.3    | 176.8     | 188.3  |
| CaMoO <sub>4</sub>                                                           |              |              |              | 131.3     | 144.9    | 153.5     | 150.6  |
| Ca <sub>3</sub> N <sub>2</sub>                                               |              |              |              | 122.2     | 140.8    | 159.2     |        |
| Ca(NO <sub>3</sub> ) <sub>2</sub>                                            | 21.4         |              |              | 173.7     | 210.5    | 243.4     |        |
| CaO                                                                          | 79.5         |              |              | 46.6      | 50.5     | 52.4      | 53.7   |
| Ca(OH) <sub>2</sub> , $\Delta H_{dec} = 99.2$                                |              |              |              | 98.4      | 107.4    |           |        |
| Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> , $\Delta H_t = 15.5^{1100}$ |              |              |              | 255.1     | 295.6    | 331.3     | 365.7  |
| CaS                                                                          | 70           |              |              | 49.2      | 51.5     | 53.0      | 54.1   |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                                  | $\Delta H_m$ | $\Delta H_v$         | $\Delta H_s$ | $C_p$    |          |          |          |
|--------------------------------------------------------------------------------------------|--------------|----------------------|--------------|----------|----------|----------|----------|
|                                                                                            |              |                      |              | 400 K    | 600 K    | 800 K    | 1000 K   |
| CaSiO <sub>3</sub> , $\Delta H_t = 7.1^{1190}$                                             | 56.1         |                      |              | 100.4    | 113.0    | 119.2    | 123.8    |
| Ca <sub>2</sub> SiO <sub>4</sub> , $\Delta H_t = 4.44^{675}$<br>$\Delta H_t = 3.26^{1420}$ |              |                      |              | 146.4    | 162.8    | 179.2    | 184.0    |
| 3CaO · SiO <sub>2</sub>                                                                    |              |                      |              | 196.4    | 218.4    | 230.8    | 240.4    |
| CaSO <sub>4</sub>                                                                          | 28.0         |                      |              | 109.7    | 129.5    | 149.2    | 169.0    |
| CaSO <sub>4</sub> · ½H <sub>2</sub> O                                                      |              |                      |              | 147.4    | 167.2    | 186.9    | 206.7    |
| CaSO <sub>4</sub> · 2H <sub>2</sub> O                                                      |              |                      |              | 260.7    | 280.3    | 300.0    | 319.8    |
| CaTiO <sub>3</sub> , $\Delta H_t = 2.30^{1257}$                                            |              |                      |              | 112.3    | 123.1    | 127.7    | 130.4    |
| Ca(VO <sub>3</sub> ) <sub>2</sub>                                                          |              |                      |              | 182.9    | 206.7    | 230.5    | 254.4    |
| CaWO <sub>4</sub>                                                                          |              |                      |              | 127.6    | 140.2    | 147.3    | 152.8    |
| Carbon                                                                                     |              |                      |              |          |          |          |          |
| C graphite                                                                                 | 117          |                      |              | 12.0     | 16.6     | 19.7     | 21.7     |
| (CN) <sub>2</sub> cyanogen                                                                 | 8.1          | 23.3                 | 19.7         | 61.9(g)  | 68.2     | 72.9     | 76.4     |
| CNBr                                                                                       |              |                      | 45.4         | 50.19(g) | 53.7     | 56.2     | 58.1     |
| CNCl                                                                                       | 11.4         |                      |              | 48.7     | 52.8     | 55.7     | 57.7     |
| CNI                                                                                        |              |                      | 59.4         | 50.8     | 53.7     | 55.8     | 57.4     |
| CO, $\Delta H_t = 0.632^{-211.6}$                                                          | 0.837        | 6.04                 |              | 29.3     | 30.4     | 31.9     | 33.2     |
| CO <sub>2</sub>                                                                            | 9.02         | 15.8                 | 25.2         | 41.3     | 47.3     | 51.4     | 54.3     |
| C <sub>2</sub> O <sub>3</sub>                                                              | 5.40         | 26.9 <sup>43.5</sup> |              | 75.0     | 85.5     | 92.7     | 97.7     |
| COCl <sub>2</sub>                                                                          | 5.74         | 24.4                 |              | 63.9     | 71.1     | 75.0     | 77.4     |
| COF <sub>2</sub>                                                                           |              | 16.1                 |              | 54.8     | 64.9     | 70.8     | 74.4     |
| COS                                                                                        | 7.73         | 18.6                 |              | 45.9     | 51.3     | 54.7     | 57.0     |
| CS <sub>2</sub>                                                                            | 4.40         | 26.7                 | 27.5         | 49.7     | 54.6     | 57.4     | 59.3     |
| Cerium                                                                                     |              |                      |              |          |          |          |          |
| Ce, $\Delta H_t = 3.01^{730}$                                                              | 5.46         | 398                  | 419          | 30.6     | 30.8     | 32.1     | 33.8     |
| CeCl <sub>3</sub>                                                                          | 54.4         | 170.1                | 326          |          |          |          |          |
| CeI <sub>3</sub>                                                                           | 51.9         |                      |              |          |          |          |          |
| CeO <sub>2</sub>                                                                           |              |                      |              | 66.9     | 69.0     | 71.1     | 73.2     |
| Cesium                                                                                     |              |                      |              |          |          |          |          |
| Cs                                                                                         | 2.09         | 63.9                 | 76.6         | 31.5     | 31.0     | 30.9(lq) | 20.8(g)  |
| CsBr                                                                                       | 23.6         | 151                  |              | 52.9     | 55.0     | 57.2(c)  | 77.4(lq) |
| CsCl, $\Delta H_t = 3.77^{470}$                                                            | 15.9         | 115.1                |              | 54.7     | 59.1     | 63.7(c)  | 77.4(lq) |
| CsF                                                                                        | 21.7         | 115.5                |              | 53.8     | 57.4     | 60.9(c)  | 74.1(lq) |
| CsI                                                                                        | 23.9         | 150.2                |              | 51.9     | 57.8(c)  | 65.5(lq) | 67.8     |
| CsIO <sub>3</sub>                                                                          | 13.0         |                      |              |          |          |          |          |
| CsOH, $\Delta H_t = 1.30^{137}$<br>$\Delta H_t = 6.1^{220}$                                | 4.56         | 120                  |              | 74.4(c)  | 81.6(lq) | 81.6     | 81.6     |
| Cs <sub>2</sub> SO <sub>4</sub> , $\Delta H_t = 4.3^{667}$                                 | 35.7         |                      | 76.5         | 112.1    | 132.2    | 163.2    | 194.2    |
| Chlorine                                                                                   |              |                      |              |          |          |          |          |
| Cl <sub>2</sub>                                                                            | 6.406        | 20.41                | 17.65        | 35.3     | 36.6     | 37.1     | 37.4     |
| ClF                                                                                        |              | 24                   |              | 33.8     | 35.6     | 36.5     | 37.0     |
| ClF <sub>3</sub>                                                                           | 7.61         | 27.5                 |              | 70.6(g)  | 76.8     | 79.4     | 80.7     |
| ClF <sub>5</sub>                                                                           |              | 22.9                 |              | 110.0    | 121.6    | 126.3    | 128.6    |
| ClO                                                                                        |              |                      |              | 33.2     | 35.3     | 36.3     | 36.9     |
| ClO <sub>2</sub>                                                                           |              | 30                   |              | 46.1     | 51.4     | 54.2     | 55.8     |
| ClO <sub>3</sub> F                                                                         | 3.83         | 19.33                |              | 75.9     | 89.2     | 96.1     | 100.0    |
| Cl <sub>2</sub> O                                                                          |              | 25.9                 |              | 51.4     | 54.7     | 56.2     | 56.9     |
| Cl <sub>2</sub> O <sub>7</sub>                                                             |              | 34.69                |              |          |          |          |          |
| Chromium                                                                                   |              |                      |              |          |          |          |          |
| Cr, $\Delta H_t = 0.0008^{38.5}$                                                           | 21.0         | 339.5                | 397          | 25.2     | 27.7     | 29.4     | 31.9     |



**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                       | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |         |          |        |
|-------------------------------------------------|--------------|--------------|--------------|----------|---------|----------|--------|
|                                                 |              |              |              | 400 K    | 600 K   | 800 K    | 1000 K |
| CrCl <sub>2</sub>                               | 32.2         | 196.7        |              | 72.6     | 77.0    | 81.5     | 85.9   |
| CrCl <sub>3</sub>                               |              |              | 237.7        | 93.1     | 99.0    | 104.9    | 110.7  |
| Cr(CO) <sub>6</sub>                             |              |              | 72.0         | 233.9    |         |          |        |
| CrN, $\Delta H_{dec} = 112$                     |              |              | 49.1         | 50.4     | 51.7    | 53.0     |        |
| CrO <sub>2</sub> Cl <sub>2</sub>                |              | 35.1         |              |          |         |          |        |
| CrO <sub>2</sub> F <sub>2</sub>                 | 23.4         | 34.3         |              |          |         |          |        |
| CrO <sub>3</sub>                                | 15.77        |              |              | 63.9     | 72.5    | 76.7     | 78.8   |
| Cr <sub>2</sub> O <sub>3</sub>                  | 129.7        |              |              | 112.7    | 120.5   | 124.3    | 127.0  |
| Cr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> |              |              |              | 316.9    | 345.2   | 373.5    | 401.8  |
| Cobalt                                          |              |              |              |          |         |          |        |
| Co, $\Delta H_t = 0.452^{427}$                  | 16.2         | 377          | 424          | 26.5     | 29.7    | 32.4     | 37.0   |
| CoCl <sub>2</sub>                               | 45           | 146          | 219          | 81.7     | 84.6    | 86.8     | 88.2   |
| CoF <sub>2</sub>                                | 59           | 202          | 315          | 75.7     | 80.8    | 82.9     | 84.2   |
| CoF <sub>3</sub>                                |              |              |              | 97       | 100     | 102      | 104    |
| CoO                                             |              |              |              | 52.9     | 54.3    | 54.8     | 56.0   |
| Co <sub>3</sub> O <sub>4</sub>                  |              |              |              | 143      | 163     | 185      | 210    |
| CoSO <sub>4</sub> , $\Delta H_t = 2.1^{691}$    |              |              |              | 119      | 141     | 152      | 158    |
| Copper                                          |              |              |              |          |         |          |        |
| Cu                                              | 13.26        | 300.4        | 337.7        | 25.3     | 26.5    | 27.4     | 28.7   |
| CuBr, $\Delta H_t = 5.86^{380}$                 | 9.6          |              |              | 56.5     | 59.8(c) | 66.9(lq) | 66.9   |
| $\Delta H_t = 2.9^{465}$                        |              |              |              |          |         |          |        |
| CuCl                                            | 10.2         | 54           | 241.8        | 56.9     | 61.5(c) | 66.9(lq) | 66.9   |
| CuCl <sub>2</sub> , $\Delta H_t = 0.700^{402}$  | 20.4         |              |              | 76.3     | 80.2(c) | 82.4(lq) | 100.0  |
| $\Delta H_t = 15.001^{598}$                     |              |              |              |          |         |          |        |
| CuCN                                            |              | 12           |              |          | 66.7    | 73.1     | 78.0   |
| CuF                                             |              |              | 268          | 55.5     | 59.6    |          |        |
| CuF <sub>2</sub>                                | 55           | 156          | 261          | 72.4     | 81.9    | 87.0     | 90.4   |
| CuI                                             | 10.9         |              |              | 55.4     | 57.8    | 60.2     | 66.9   |
| CuO                                             | 11.8         |              |              | 46.8     | 50.8    | 53.2     | 55.0   |
| Cu <sub>2</sub> O                               | 64.8         |              |              | 67.6     | 73.3    | 77.6     | 81.5   |
| CuS                                             |              |              |              | 48.8     | 51.0    | 53.2     | 55.4   |
| Cu <sub>2</sub> S, $\Delta H_t = 3.85^{103}$    | 10.9         |              |              | 97.3     | 97.3    | 85.0     | 85.0   |
| $\Delta H_t = 0.84^{350}$                       |              |              |              |          |         |          |        |
| Cu <sub>2</sub> Se, $\Delta H_t = 4.85^{110}$   |              |              |              | 90.9     | 91.7    | 92.5     | 93.4   |
| CuSO <sub>4</sub>                               |              |              |              | 114.9    | 136.3   | 147.7    | 153.8  |
| Dysprosium                                      |              |              |              |          |         |          |        |
| Dy                                              | 11.06        | 280          | 290.4        |          |         |          |        |
| Erbium                                          |              |              |              |          |         |          |        |
| Er                                              | 19.90        | 280          | 317.2        |          |         |          |        |
| Europium                                        |              |              |              |          |         |          |        |
| Eu                                              | 9.21         | 176          | 178          |          |         |          |        |
| Fluorine                                        |              |              |              |          |         |          |        |
| F <sub>2</sub> , $\Delta H_t = 0.728^{-227.6}$  | 0.510        | 6.62         |              | 33.0     | 35.2    | 36.3     | 37.1   |
| FNO <sub>3</sub>                                |              |              |              | 75.1     | 87.8    | 94.8     | 98.9   |
| Gadolinium                                      |              |              |              |          |         |          |        |
| Gd                                              | 10.05        | 301.3        |              | 36.6     | 35.5    | 34.5     | 33.5   |
| Gd <sub>2</sub> O <sub>3</sub>                  |              |              |              | 113.4    | 120.1   | 124.4    | 127.9  |
| Gallium                                         |              |              |              |          |         |          |        |
| Ga                                              | 5.59         | 254          |              | 27.1(lq) | 26.7    | 26.6     | 26.6   |
| GaBr <sub>3</sub>                               | 12.1         | 38.9         |              |          |         |          |        |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                     | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$   |         |          |        |
|-----------------------------------------------|--------------|--------------|--------------|---------|---------|----------|--------|
|                                               |              |              |              | 400 K   | 600 K   | 800 K    | 1000 K |
| GaCl <sub>3</sub>                             | 11.13        | 23.9         |              |         |         |          |        |
| GaI <sub>3</sub>                              | 12.9         | 56.5         |              |         |         |          |        |
| Ga <sub>2</sub> O <sub>3</sub>                | 100          |              |              | 91.4    | 112.5   | 133.5    |        |
| GaSb                                          | 25.1         |              |              |         |         |          |        |
| Germanium                                     |              |              |              |         |         |          |        |
| Ge, $\Delta H_t = 37.03^{938.3}$              | 36.94        | 334          |              | 24.3    | 25.4    | 26.2     | 26.9   |
| GeBr <sub>4</sub>                             |              | 41.4         |              |         |         |          |        |
| GeCl <sub>4</sub>                             |              | 27.9         |              | 100.7   | 104.6   | 106.1    | 106.8  |
| GeH <sub>4</sub>                              |              | 14.1         |              |         |         |          |        |
| Ge <sub>2</sub> H <sub>6</sub>                |              | 25.1         |              |         |         |          |        |
| Ge <sub>3</sub> H <sub>8</sub>                |              | 32.2         |              |         |         |          |        |
| GeO <sub>2</sub>                              | 43.9         |              |              | 61.39   | 69.1    | 72.4     | 75.0   |
| Gold                                          |              |              |              |         |         |          |        |
| Au                                            | 12.55        | 324          |              | 25.8    | 26.8    | 27.8     | 28.8   |
| AuSn                                          | 25.6         |              |              | 54.1    | 63.3(c) | 60.6(lq) |        |
| Hafnium                                       |              |              |              |         |         |          |        |
| Hf, $\Delta H_t = 5.9^{1750}$                 | 27.2         | 571          | 618.4        | 26.7    | 28.6    | 30.3     | 31.9   |
| HfCl <sub>4</sub>                             | 75           |              | 99.6         | 125.4   | 105.8   | 106.7    | 107.1  |
| HfO <sub>2</sub> , $\Delta H_t = 10.5^{1700}$ | 104.6        |              |              | 67.7    | 73.9    | 77.3     | 79.9   |
| Helium                                        |              |              |              |         |         |          |        |
| He                                            | 0.0138       | 0.0829       |              | 20.79   | 20.79   | 20.79    | 20.79  |
| Holmium                                       |              |              |              |         |         |          |        |
| Ho                                            | 16.8         | 71           |              | 280     | 317     |          |        |
| Hydrogen                                      |              |              |              |         |         |          |        |
| H <sub>2</sub>                                | 0.117        | 0.904        |              | 29.2    | 29.3    | 29.6     | 30.2   |
| <sup>1</sup> H <sup>2</sup> H                 |              |              |              | 29.2    | 29.4    | 29.9     | 30.7   |
| <sup>2</sup> H <sub>2</sub>                   |              |              |              | 29.2    | 29.6    | 30.5     | 31.6   |
| HBO <sub>2</sub>                              | 14.3         |              | 242.1        | 61.5(c) |         |          |        |
| H <sub>3</sub> BO <sub>3</sub>                | 22.3         |              |              |         |         |          |        |
| HBr                                           | 2.406        | 17.61        | 12.7         | 29.2    | 29.8    | 31.1     | 32.3   |
| HCl, $\Delta H_t = 1.188^{-174.77}$           | 1.992        | 16.14        | 9.1          | 19.2    | 29.2    | 29.6     | 31.6   |
| <sup>2</sup> HCl                              |              |              |              | 29.4    | 30.6    | 32.1     | 33.5   |
| HCIO                                          |              |              |              | 40.0    | 44.0    | 46.6     | 48.5   |
| HCN                                           | 8.406        | 25.22        |              | 39.4    | 44.2    | 47.9     | 51.0   |
| HF                                            | 4.58         |              |              | 29.1    | 29.2    | 29.5     | 30.2   |
| <sup>2</sup> HF                               |              |              |              | 29.2    | 29.5    | 30.5     | 31.6   |
| H <sub>2</sub> F <sub>2</sub> dimer           |              |              |              | 49.7    | 56.5    | 61.0     | 64.4   |
| HFO                                           |              |              |              | 38.6    | 42.8    | 45.7     | 47.9   |
| HI                                            | 2.87         | 19.77        | 17.4         | 29.3    | 30.3    | 31.8     | 33.1   |
| HNCO isocyanic acid                           |              |              |              | 50.6    | 58.3    | 63.5     | 67.5   |
| HNCS isothiocyanic acid                       |              |              |              | 53.2    | 61.0    | 65.9     | 69.3   |
| HNO <sub>2</sub> <i>cis</i>                   |              |              |              | 51.4    | 59.9    | 65.4     | 69.2   |
| <i>trans</i>                                  |              |              |              | 52.1    | 60.3    | 65.6     | 69.3   |
| HNO <sub>3</sub>                              | 10.47        | 39.46        | 39.1         | 63.1    | 76.8    | 85.0     | 90.4   |
| HN <sub>3</sub>                               |              | 30.5         |              |         |         |          |        |
| H <sub>2</sub> O                              | 6.009        | 40.66        | 44.0         | 34.3(g) | 36.4    | 38.8     | 41.4   |
| <sup>1</sup> H <sup>2</sup> HO                |              |              |              | 34.8    | 37.5    | 40.4     | 43.3   |
| <sup>2</sup> H <sub>2</sub> O                 |              |              |              | 35.6    | 38.8    | 42.2     | 45.4   |
| H <sub>2</sub> O <sub>2</sub>                 | 12.50        |              | 51.63        | 48.5    | 55.7    | 59.8     | 66.7   |
| <sup>2</sup> H <sub>2</sub> O <sub>2</sub>    | 12.68        |              | 52.4         |         |         |          |        |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |           |          |           |
|--------------------------------------------------------------|--------------|--------------|--------------|----------|-----------|----------|-----------|
|                                                              |              |              |              | 400 K    | 600 K     | 800 K    | 1000 K    |
| HPH <sub>2</sub> O <sub>2</sub>                              | 9.67         |              |              |          |           |          |           |
| H <sub>3</sub> PO <sub>3</sub>                               | 12.84        |              |              |          |           |          |           |
| H <sub>3</sub> PO <sub>4</sub>                               | 13.4         |              |              | 175.7    | 236.0     | 296.2    | 365.5     |
| H <sub>2</sub> S, $\Delta H_t = 1.531^{-169.61}$             | 23.8         | 18.67        | 14.1         | 38.9     | 42.5      | 45.8     |           |
| H <sub>2</sub> S <sub>2</sub>                                |              | 33.8         |              |          |           |          |           |
| H <sub>2</sub> Se                                            |              | 19.7         |              |          |           |          |           |
| HSO <sub>3</sub> F                                           |              |              |              | 87.5     | 102.6     | 111.0    | 116.3     |
| H <sub>2</sub> SO <sub>4</sub>                               | 10.71        | 50.2         |              | 158.2    | 197.0(lq) | 125.9(g) | 132.7     |
| H <sub>2</sub> SO <sub>4</sub> · H <sub>2</sub> O            | 19.46        |              |              | 228.5    |           |          |           |
| H <sub>2</sub> SO <sub>4</sub> · 2H <sub>2</sub> O           | 18.24        |              |              | 294.6    |           |          |           |
| H <sub>2</sub> SO <sub>4</sub> · 3H <sub>2</sub> O           | 24.0         |              |              | 347.8    |           |          |           |
| H <sub>2</sub> SO <sub>4</sub> · 4H <sub>2</sub> O           | 30.64        |              |              | 410.3    |           |          |           |
| H <sub>2</sub> Te                                            |              | 19.2         |              |          |           |          |           |
| Indium                                                       |              |              |              |          |           |          |           |
| In                                                           | 3.28         | 231.8        | 243.1        | 28.5(c)  | 30.1(lq)  | 30.1     | 30.1      |
| InBr                                                         | 15           | 92           |              |          |           |          |           |
| InBr <sub>3</sub>                                            | 26           |              |              |          |           |          |           |
| InCl                                                         | 21.3         |              |              |          |           |          |           |
| InCl <sub>3</sub>                                            | 27           |              |              |          |           |          |           |
| InF <sub>3</sub>                                             | 64           |              |              |          |           |          |           |
| InI                                                          | 17.3         | 90.8         |              |          |           |          |           |
| InI <sub>3</sub>                                             | 18.5         |              |              |          |           |          |           |
| In <sub>2</sub> O <sub>3</sub>                               | 105          |              |              |          |           |          |           |
| InSb                                                         | 25.5         |              |              |          |           |          |           |
| Iodine                                                       |              |              |              |          |           |          |           |
| I <sub>2</sub>                                               | 150.66       | 41.6         | 62.4         | 79.6(lq) | 37.6(g)   | 37.9     | 38.1      |
| ICl                                                          | 11.60        |              | 52.9         | 98.3(lq) | 90.0      | 81.6     | 73.2      |
| IF                                                           |              |              |              | 35.1     | 36.6      | 37.3     | 37.7      |
| IF <sub>5</sub>                                              |              | 41.3         |              | 476.1(g) | 516.7     | 533.0    | 541.4     |
| IF <sub>7</sub>                                              |              |              |              | 152.0(g) | 167.6     | 173.9    | 177.0     |
| Iridium                                                      |              |              |              |          |           |          |           |
| Ir                                                           | 41.12        | 231.8        | 243.1        | 28.5(c)  | 30.1(lq)  | 30.1     | 30.1      |
| IrF <sub>6</sub>                                             | 8.40         | 36           |              |          |           |          |           |
| IrO <sub>2</sub>                                             |              |              |              | 63.8     | 76.5      | 89.2     | 102.0     |
| Iron                                                         |              |              |              |          |           |          |           |
| Fe, $\Delta H_t = 0.90^{911}$<br>$\Delta H_t = 0.837^{1392}$ | 13.81        | 340          | 415.5        | 27.4     | 32.1      | 38.0     | 54.4      |
| FeBr <sub>2</sub>                                            | 50.2         |              |              |          |           |          |           |
| FeBr <sub>3</sub> , $\Delta H_t = 0.418^{377}$               | 50.2         |              | 207.5        | 83.0     | 87.0      | 91.4     | 95.9      |
| Fe <sub>2</sub> C, $\Delta H_t = 0.75^{190}$                 | 51.5         |              |              | 115.7    | 114.7     | 117.2    | 119.8     |
| FeCl <sub>2</sub>                                            | 43.01        | 26.3         |              | 79.7     | 83.1      | 85.5     | 101.2     |
| FeCl <sub>3</sub>                                            | 43.1         | 43.76        |              | 106.7(c) | 133.9(lq) | 82.3(g)  | 81.5      |
| FeCO <sub>3</sub>                                            |              |              |              | 93.5     | 115.9     | 138.3    |           |
| Fe(CO) <sub>5</sub>                                          | 13.23        | 33.72        |              | 189.0    | 209.8     | 223.1    | 232.2     |
| FeCr <sub>2</sub> O <sub>4</sub>                             |              |              |              | 152.0    | 167.7     | 175.9    | 182.2     |
| FeF <sub>2</sub>                                             | 51.9         | 224.4        | 316          | 72.0     | 77.1      | 80.3     | 82.1      |
| FeF <sub>3</sub>                                             |              |              | 274          | 96.4     | 96.8      | 99.3     | 101.8     |
| FeI <sub>2</sub> , $\Delta H_t = 0.8^{377}$                  | 45           | 104.6        | 192          | 83.9     | 84.4      | 110.9    | 113.0(lq) |
| Fe <sub>3</sub> N                                            |              |              |              | 72.6     | 77.7      | 82.8     | 87.9      |
| FeO                                                          | 24.06        |              |              | 51.8     | 54.9      | 57.3     | 59.4      |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                            | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$   |          |           |          |
|------------------------------------------------------|--------------|--------------|--------------|---------|----------|-----------|----------|
|                                                      |              |              |              | 400 K   | 600 K    | 800 K     | 1000 K   |
| $\text{Fe}_2\text{O}_3$ , $\Delta H_t = 0.67^{677}$  |              |              |              | 120.1   | 141.2    | 158.2     | 150.6    |
| $\text{Fe}_3\text{O}_4$                              | 138.1        |              |              | 171.1   | 212.5    | 252.9     |          |
| $\text{Fe}(\text{OH})_2$                             |              |              | 243.5        | 102.1   | 111.3    | 118.9     | 123.4    |
| $\text{Fe}(\text{OH})_3$                             |              |              |              | 118.0   | 140.6    | 154.8     | 164.9    |
| $\text{FeS}$ , $\Delta H_t = 0.40^{138}$             | 31.5         |              |              | 89.2    | 62.0     | 58.6      | 59.0     |
| $\Delta H_t = 0.095^{325}$                           |              |              |              |         |          |           |          |
| $\text{FeS}_2$ marcasite                             |              |              |              | 69.2    | 74.6     | 78.7      | 82.8     |
| pyrite                                               |              |              |              | 68.9    | 74.3     | 78.3      | 82.5     |
| $\text{FeSiO}_3$                                     |              |              |              | 100.8   | 114.3    | 124.5     | 133.9    |
| $\text{Fe}_2\text{SiO}_4$                            | 92           |              |              | 150.9   | 168.5    | 179.7     | 189.1    |
| $\text{FeSO}_4$                                      |              |              |              | 116.7   | 138.0    | 149.4     |          |
| $\text{Fe}_2(\text{SO}_4)_3$                         |              |              |              | 307.0   | 363.3    | 393.3     | 409.2    |
| $\text{FeTiO}_3$ ilmenite                            | 90.8         | 111.4        | 122.0        | 128.1   | 132.8    |           |          |
| Krypton                                              |              |              |              |         |          |           |          |
| Kr                                                   | 1.37         | 9.08         |              |         |          |           |          |
| Lanthanum                                            |              |              |              |         |          |           |          |
| La, $\Delta H_t = 2.85^{868}$                        | 6.20         | 402.1        |              | 28.5    | 29.8     | 31.2      | 32.5     |
| $\text{LaCl}_3$                                      | 43.1         | 192.1        |              | 105.8   | 110.1    | 114.3     | 118.7    |
| $\text{La}_2\text{O}_3$                              |              |              |              | 117.3   | 124.7    | 128.9     | 132.3    |
| Lead                                                 |              |              |              |         |          |           |          |
| Pb                                                   | 4.77         | 179.5        | 195.2        | 27.7    | 29.4     | 30.0      | 29.4     |
| $\text{Pb}(\text{BO}_2)_2$                           |              |              |              | 129.7   | 162.3    |           |          |
| $\text{PbB}_4\text{O}_7$                             |              |              |              | 207     | 265      | 305       | 330      |
| $\text{PbBr}_2$                                      | 16.44        | 133          | 173          | 81.3    | 88.8     | 112.1(lq) | 112.1    |
| $\text{Pb}(\text{CH}_3)_4$                           | 10.86        |              |              |         |          |           |          |
| $\text{Pb}(\text{C}_2\text{H}_5)_4$                  | 8.80         |              |              |         |          |           |          |
| $\text{PbCl}_2$                                      | 21.9         | 127          | 185.3        | 80.1    | 85.9     | 111.5(lq) | 111.5    |
| $\text{PbCO}_3$                                      |              |              |              | 99.7    | 123.6    | 147.6     |          |
| $\text{PbF}_2$ , $\Delta H_t = 1.46^{310}$           | 14.7         | 157          |              | 76.1    | 82.5     | 89.1      | 95.6     |
| $\text{PbI}_2$                                       | 23.4         | 104          | 172          | 78.9    | 83.7(c)  | 108.6(lq) | 108.6    |
| $\text{PbMoO}_4$                                     |              |              |              | 135.3   | 148.9    | 159.0     | 168.2    |
| $\text{PbO}$ , $\Delta H_t = 0.17^{488}$             | 25.5         | 207          |              | 50.4    | 55.4     | 55.0      | 57.8     |
| $\text{PbO}_2$                                       |              |              |              | 67.6    |          |           |          |
| $\text{Pb}_3\text{O}_4$                              |              |              |              | 173.1   | 190.8    | 199.2     |          |
| PbS                                                  | 18.8         | 230          |              | 50.5    | 52.4     | 54.3      | 56.2     |
| $\text{PbSiO}_3$                                     | 26.0         |              |              | 101.5   | 113.5    | 125.6     | 138.4    |
| $\text{Pb}_2\text{SiO}_4$                            | 51.0         |              |              | 152.0   | 173.3    | 184.2     | 189.1    |
| $\text{PbSO}_4$ , $\Delta H_t = 17.2^{866}$          | 40.2         |              |              | 108.7   | 128.6    | 152.4     | 177.3    |
| $\text{PbSO}_4 \cdot \text{PbO}$                     |              |              |              | 157.3   | 182.5    | 211.7     | 242.0    |
| Lithium                                              |              |              |              |         |          |           |          |
| Li                                                   | 3.00         | 147.1        | 159.3        | 27.6(c) | 29.5(lq) | 28.9      | 28.8     |
| $\text{Li}_2\text{AlF}_6$ , $\Delta H_t = 9.5^{562}$ | 110.5        |              |              | 236.4   | 262.8    | 290.8     | 318.6    |
| $\text{LiAlO}_2$                                     | 87           |              |              | 81.5    | 92.7     | 98.2      | 102.0    |
| $\text{LiBH}_4$                                      |              |              |              | 91.0    |          |           |          |
| $\text{LiBeF}_3$                                     | 27.2         |              |              | 104.6   | 129.7(c) | 159.0(lq) | 159.0    |
| $\text{Li}_2\text{BeF}_4$                            | 44.0         |              |              | 150.5   | 180.2(c) | 232.1(lq) | 232.1    |
| $\text{LiBO}_2$                                      | 33.8         | 265          |              | 81.1    | 85.1     | 96.9      | 108.3    |
| $\text{Li}_2\text{B}_4\text{O}_7$                    | 121          |              |              | 197.6   | 241.1    | 274.4     | 300.2    |
| LiBr                                                 | 17.6         | 107.1        |              | 51.3    | 56.1     | 64.5(c)   | 65.3(lq) |
| LiCl                                                 | 19.9         |              |              | 51.0    | 55.6     | 65.8      |          |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                                  | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |           |          |           |
|--------------------------------------------------------------------------------------------|--------------|--------------|--------------|----------|-----------|----------|-----------|
|                                                                                            |              |              |              | 400 K    | 600 K     | 800 K    | 1000 K    |
| LiClO <sub>4</sub>                                                                         | 29           |              |              | 130.0(c) | 161.0(lq) | 161      | 161       |
| Li <sub>2</sub> CO <sub>3</sub> , $\Delta H_t = 0.561^{350}$<br>$\Delta H_t = 2.238^{410}$ | 41           |              |              | 112.2    | 149.4     | 159.0    |           |
| LiF                                                                                        | 27.09        | 146.8        | 276.1        | 46.5     | 51.6      | 55.7     | 59.6      |
| LiH                                                                                        | 22.6         |              | 231.3        | 34.8     | 46.4      | 57.3     |           |
| LiI                                                                                        | 14.6         |              |              |          |           |          |           |
| LiIO <sub>3</sub> , $\Delta H_t = 2.22^{260}$                                              |              |              |              |          |           |          |           |
| Li <sub>3</sub> N                                                                          |              |              |              | 87.1     | 106.4     | 124.4    | 141.0     |
| LiNO <sub>3</sub>                                                                          | 24.9         |              |              |          |           |          |           |
| Li <sub>2</sub> O                                                                          | 58.6         |              |              | 64.0     | 73.8      | 80.6     | 86.2      |
| Li <sub>2</sub> O <sub>2</sub>                                                             |              |              |              | 82.7(c)  | 80.2(g)   | 81.4     | 82.1      |
| LiOH                                                                                       | 20.88        | 187.9        | 250.6        | 58.0     | 68.2(c)   | 87.1(lq) | 87.1      |
| Li <sub>2</sub> SiO <sub>3</sub>                                                           | 28.0         |              |              | 118.8    | 134.3     | 144.4    | 152.3     |
| Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> , $\Delta H_t = 0.941^{936}$                | 53.8         |              |              | 174.9    | 205.7     | 222.6    | 235.4     |
| Li <sub>2</sub> SO <sub>4</sub> , $\Delta H_t = 28.5^{575}$                                | 7.50         |              |              | 139.2    | 168.5     | 196.1    | 223.4     |
| Li <sub>2</sub> TiO <sub>3</sub> , $\Delta H_t = 11.51^{1212}$                             | 110.7        |              |              | 127.4    | 141.5     | 149.0    | 153.9     |
| Lutetium                                                                                   |              |              |              |          |           |          |           |
| Lu                                                                                         | (22)         | 414          |              |          |           |          |           |
| Magnesium                                                                                  |              |              |              |          |           |          |           |
| Mg                                                                                         | 8.48         | 128          | 147          | 26.1     | 28.2      | 30.5     |           |
| MgAl <sub>2</sub> O <sub>4</sub>                                                           | 192          |              |              | 138.0    | 157.9     | 169.5    | 178.7     |
| MgBr <sub>2</sub>                                                                          | 39.3         | 149          | 222          | 77.3     | 81.4      | 84.5     |           |
| MgCl <sub>2</sub>                                                                          | 43.1         | 156.2        | 249.2        | 75.7     | 79.9      | 82.5     |           |
| MgCO <sub>3</sub>                                                                          | 59           |              |              | 89.9     | 109.0     | 122.3    | 131.8     |
| MgF <sub>2</sub>                                                                           | 58.5         | 274.1        | 399.5        | 68.5     | 75.3      | 78.6     | 80.5      |
| MgH <sub>2</sub>                                                                           | 14           |              |              |          |           |          |           |
| MgI <sub>2</sub>                                                                           | 26           |              | 206          | 78.4     | 83.0      | 96.3(c)  | 100.4(lq) |
| Mg <sub>3</sub> N <sub>2</sub> , $\Delta H_t = 0.46^{550}$<br>$\Delta H_t = 0.92^{788}$    |              |              | 107.6        | 113.8    | 119.9     | 123.8    |           |
| Mg(NO <sub>3</sub> ) <sub>2</sub>                                                          |              |              |              | 168.5    | 225.5     |          |           |
| MgO                                                                                        | 77           |              |              | 42.6     | 47.4      | 49.7     | 51.2      |
| Mg(OH) <sub>2</sub>                                                                        |              |              |              | 91.7     |           |          |           |
| Mg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>                                            | 121          |              |              | 240.2    | 282.2     | 320.6    | 351.5     |
| MgS                                                                                        | 63           |              |              |          |           |          |           |
| Mg <sub>2</sub> Si                                                                         | 85.8         |              |              | 73.8     | 79.8      | 83.9     | 87.4      |
| MgSiO <sub>3</sub> , $\Delta H_t = 0.67^{630}$<br>$\Delta H_t = 1.63^{985}$                | 71           |              |              | 94.2     | 107.0     | 115.8    | 120.3     |
| Mg <sub>2</sub> SiO <sub>4</sub>                                                           |              |              |              | 137.6    | 156.4     | 167.1    | 174.6     |
| MgSO <sub>4</sub>                                                                          | 14.6         |              |              | 110.0    | 127.6     | 140.5    | 151.7     |
| MgTiO <sub>3</sub>                                                                         |              |              |              | 105.2    | 118.5     | 125.4    | 129.9     |
| Mg <sub>2</sub> TiO <sub>4</sub>                                                           |              |              |              | 146      | 164       | 175      | 184       |
| MgWO <sub>4</sub>                                                                          |              |              |              | 123.4    | 137.0     | 146.1    | 154.8     |
| Manganese                                                                                  |              |              |              |          |           |          |           |
| Mn, $\Delta H_t = 2.23^{727}$<br>$\Delta H_t = 2.12^{1101}$<br>$\Delta H_t = 1.88^{1137}$  | 12.9         | 221          |              | 28.5     | 31.9      | 34.9     | 37.5      |
| MnBr <sub>2</sub>                                                                          | 33           | 113          |              | 77.8     | 82.8      | 87.7     |           |
| Mn <sub>3</sub> C, $\Delta H_t = 14.94^{1037}$                                             |              |              |              | 104.4    | 115.0     | 121.7    | 127.4     |
| MnCl <sub>2</sub>                                                                          | 30.7         | 149.0        |              | 77.2     | 81.8      | 85.1     | 96.2(lq)  |
| Mn <sub>2</sub> (CO) <sub>10</sub>                                                         |              |              | 62.8         |          |           |          |           |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |           |         |           |
|--------------------------------------------------------------|--------------|--------------|--------------|----------|-----------|---------|-----------|
|                                                              |              |              |              | 400 K    | 600 K     | 800 K   | 1000 K    |
| MnF <sub>2</sub>                                             | 23.0         |              |              | 70.6     | 75.7      | 80.7    | 85.9      |
| MnI <sub>2</sub>                                             | 42           |              |              | 78.1     | 83.6      | 89.0    | 108.8     |
| MnO                                                          | 54.4         |              |              | 47.5     | 50.3      | 52.4    | 54.2      |
| MnO <sub>2</sub>                                             |              |              |              | 63.4     | 71.1      | 75.1    |           |
| Mn <sub>2</sub> O <sub>3</sub>                               |              |              |              | 109.0    | 120.8     | 129.4   | 137.2     |
| Mn <sub>3</sub> O <sub>4</sub> , $\Delta H_t = 20.79^{1172}$ |              |              |              | 157.3    | 169.5     | 179.7   | 189.3     |
| MnS                                                          | 26.4         |              |              | 50.7     | 52.2      | 53.7    | 55.2      |
| MnSiO <sub>3</sub>                                           | 66.9         |              |              | 100.9    | 113.1     | 119.5   | 124.2     |
| MnSO <sub>4</sub>                                            |              |              |              | 119.0    | 136.7     | 147.7   |           |
| MnTiO <sub>3</sub>                                           |              |              |              | 111.7    | 121.2     | 125.7   | 128.8     |
| Mercury                                                      |              |              |              |          |           |         |           |
| Hg                                                           | 2.29         | 59.1         | 61.4         | 27.4     | 27.1(lq)  | 20.8(g) | 20.8      |
| HgBr <sub>2</sub>                                            | 17.9         | 58.9         |              | 78.3     | 102.1(lq) | 102.1   | 102.1     |
| Hg <sub>2</sub> Br <sub>2</sub>                              |              |              |              | 109.6    | 115.6     |         |           |
| HgCl <sub>2</sub>                                            | 19.41        | 58.9         |              | 77.0(c)  | 102.9(lq) |         |           |
| Hg <sub>2</sub> Cl <sub>2</sub>                              |              |              |              | 106.0    | 112.1     |         |           |
| HgF <sub>2</sub>                                             | 23.0         | 92           |              | 77.0     | 81.2      | 85.4(c) | 102.9(lq) |
| Hg <sub>2</sub> F <sub>2</sub>                               |              |              |              | 104.7    | 111.7     | 116.9   |           |
| HgI <sub>2</sub> , $\Delta H_t = 2.52^{129}$                 | 18.9         | 59.2         |              | 82.0(c)  | 84.1(lq)  | 62.2(g) | 62.2      |
| Hg <sub>2</sub> I <sub>2</sub>                               | 27.8         |              |              | 110.4(c) | 136.4(lq) |         |           |
| HgO                                                          |              |              |              | 48.3     | 54.1      |         |           |
| HgS, $\Delta H_t = 4.2^{386}$                                |              |              |              | 48.0     | 51.0      | 54.1    |           |
| Molybdenum                                                   |              |              |              |          |           |         |           |
| Mo                                                           | 37.48        | 617          | 664          | 25.1     | 26.5      | 27.4    | 28.4      |
| MoBr <sub>3</sub>                                            |              |              |              | 106.9    | 109.8     | 112.7   |           |
| MoCl <sub>4</sub>                                            | 17           | 61.5         |              | 135.0(c) | 146.4(lq) |         |           |
| MoCl <sub>5</sub>                                            | 18.8         | 62.8         |              | 167.4(c) | 175.7(lq) | 175.7   | 175.7     |
| Mo(CO) <sub>6</sub>                                          |              | 72.5         | 69.9         |          |           |         |           |
| MoF <sub>6</sub> , $\Delta H_t = 8.17^{-9.65}$               | 4.33         | 27.2         | 28.0         | 133.1    | 145.3     | 150.4   | 153.0     |
| MoO <sub>2</sub>                                             |              |              |              | 63.5     | 71.2      | 76.5    | 81.4      |
| MoO <sub>3</sub>                                             | 48           | 138          |              | 83.1     | 91.8      | 100.0   | 109.0     |
| MoS <sub>2</sub>                                             |              |              |              | 68.9     | 73.6      | 76.2    | 78.2      |
| Mo <sub>2</sub> S <sub>3</sub>                               | 130          |              |              | 117.5    | 127.4     | 135.2   | 142.3     |
| Neodymium                                                    |              |              |              |          |           |         |           |
| Nd, $\Delta H_t = 2.98^{862}$                                | 7.14         | 289          |              | 28.2     | 32.1      | 36.9    | 42.0      |
| Nd <sub>2</sub> O <sub>3</sub>                               |              |              |              | 120.3    | 130.0     | 137.7   | 144.4     |
| Neon                                                         |              |              |              |          |           |         |           |
| Ne                                                           | 0.335        | 1.71         |              |          |           |         |           |
| Neptunium                                                    |              |              |              |          |           |         |           |
| Np, $\Delta H_t = 8.37^{280}$                                | 3.20         | 336          |              | 34.8     |           |         |           |
| Nickel                                                       |              |              |              |          |           |         |           |
| Ni                                                           | 17.48        | 377.5        |              | 28.5     | 30.0      | 31.0    | 32.2      |
| NiCl <sub>2</sub>                                            | 71.2         |              | 231.0        | 76.3     | 79.9      | 80.9    |           |
| Ni(CO) <sub>4</sub>                                          | 13.8         | 29.3         |              | 160.4(g) | 173.2     | 182.1   | 188.6     |
| NiF <sub>2</sub>                                             |              |              |              | 76.4     | 78.5      | 82.6    |           |
| NiO                                                          |              |              |              | 52.2     | 51.8      | 53.6    | 55.2      |
| NiS, $\Delta H_t = 6.4^{379}$                                | 30.1         |              |              | 12.1     | 13.2      | 13.7    | 15.1      |
| Ni <sub>3</sub> S <sub>2</sub> , $\Delta H_t = 56.2^{556}$   | 19.7         |              |              | 127.1    | 139.9     | 150.7   | 188.6     |
| NiS <sub>2</sub>                                             | 65.7         |              |              | 72.8     | 70.0      | 81.0    | 85.2      |
| NiSO <sub>4</sub>                                            |              |              |              | 142.6    | 150.8     | 159.2   | 167.4     |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                         | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |           |       |        |
|-----------------------------------------------------------------------------------|--------------|--------------|--------------|----------|-----------|-------|--------|
|                                                                                   |              |              |              | 400 K    | 600 K     | 800 K | 1000 K |
| NiWO <sub>4</sub>                                                                 |              |              |              | 138.9    | 144.6     | 150.3 | 155.9  |
| Niobium                                                                           |              |              |              |          |           |       |        |
| Nb                                                                                | 30           | 689.9        | 726          | 25.4     | 26.3      | 27.2  | 28.0   |
| NbBr <sub>5</sub>                                                                 | 24.0         | 50.2         | 112.5        | 147.9(c) | 147.9(lq) |       |        |
| NbCl <sub>5</sub>                                                                 | 38.3         | 52.7         |              | 170.7(c) | 127.9(g)  | 129.8 | 130.7  |
| NbF <sub>5</sub>                                                                  | 12.2         | 52.3         |              | 43.5(lq) |           |       |        |
| NbI <sub>5</sub>                                                                  | 37.7         | 58.6         |              | 182.0(c) |           |       |        |
| NbN, $\Delta H_t = 4.2^{1370}$                                                    | 46.0         |              |              | 45.4     | 49.9      | 51.6  | 53.2   |
| NbO                                                                               | 85           | 618          |              | 44.0     | 47.2      | 49.5  | 51.5   |
| NbO <sub>2</sub> , $\Delta H_t = 3.42^{817}$                                      | 92           |              | 598.0        | 63.5     | 71.7      | 70.5  | 87.5   |
| Nb <sub>2</sub> O <sub>5</sub>                                                    | 104.3        |              |              | 145.0    | 160.7     | 170.0 | 175.5  |
| Nitrogen                                                                          |              |              |              |          |           |       |        |
| N <sub>2</sub> , $\Delta H_t = 0.230^{-237.53}$                                   | 0.720        | 5.577        |              | 29.2     | 30.1      | 31.4  | 32.7   |
| NF <sub>3</sub>                                                                   |              | 11.6         |              | 61.9     | 71.4      | 76.0  | 78.4   |
| N <sub>2</sub> F <sub>2</sub> <i>cis</i>                                          | 15.4         | 91.6         |              | 58.2     | 68.3      | 73.6  | 76.6   |
| <i>trans</i>                                                                      | 14.2         | 87.9         |              | 60.2     | 68.9      | 73.8  | 76.7   |
| N <sub>2</sub> F <sub>4</sub>                                                     |              | 13.3         |              |          |           |       |        |
| NH <sub>3</sub> (see Ammonium)                                                    |              |              |              |          |           |       |        |
| N <sub>2</sub> H <sub>4</sub>                                                     | 12.66        | 41.8         | 44.7         | 61.7(g)  | 77.6      | 88.2  | 96.4   |
| NO                                                                                | 2.30         | 13.83        |              | 29.9     | 31.2      | 32.8  | 34.0   |
| NOCl                                                                              |              | 25.8         |              | 47.1     | 50.7      | 53.2  | 54.9   |
| NOF                                                                               |              | 19.3         |              | 44.6     | 48.9      | 51.7  | 53.5   |
| NOF <sub>3</sub>                                                                  |              |              |              | 78.7     | 90.9      | 97.0  | 100.5  |
| NO <sub>2</sub>                                                                   |              |              |              | 40.5     | 46.4      | 50.4  | 53.0   |
| NO <sub>2</sub> Cl                                                                |              | 25.7         |              | 59.6     | 68.1      | 73.1  | 76.1   |
| NO <sub>2</sub> F                                                                 |              | 18.0         |              | 57.0     | 66.4      | 71.9  | 75.3   |
| NO <sub>3</sub>                                                                   |              |              |              | 55.9     | 67.4      | 73.3  | 76.5   |
| N <sub>2</sub> O                                                                  | 6.54         | 16.53        |              | 42.7     | 48.4      | 52.2  | 54.9   |
| N <sub>2</sub> O <sub>4</sub>                                                     | 14.65        | 38.12        |              | 88.5     | 104.0     | 113.4 | 119.2  |
| N <sub>2</sub> O <sub>5</sub>                                                     |              |              | 62.3         | 110.9    | 128.4     | 137.0 | 141.4  |
| NSF                                                                               |              | 22.2         |              |          |           |       |        |
| Osmium                                                                            |              |              |              |          |           |       |        |
| Os                                                                                | 57.85        | 738          |              | 25.1     | 25.9      | 26.7  | 27.4   |
| OsF <sub>6</sub>                                                                  |              | 28.62        |              |          |           |       |        |
| OsO <sub>4</sub>                                                                  | 9.8          | 39.54        |              |          |           |       |        |
| Oxygen                                                                            |              |              |              |          |           |       |        |
| O <sub>2</sub> , $\Delta H_t = 0.092^{-249.49}$<br>$\Delta H_t = 0.745^{-229.38}$ | 0.444        | 6.820        | 8.204        | 30.11    | 32.09     | 33.74 | 34.88  |
| O <sub>3</sub>                                                                    |              | 10.84        |              | 43.74    | 49.86     | 53.15 | 55.02  |
| OF <sub>2</sub>                                                                   |              | 11.09        |              | 64.3     | 72.4      | 76.4  | 78.6   |
| O <sub>2</sub> F <sub>2</sub>                                                     |              | 19.1         |              |          |           |       |        |
| Palladium                                                                         |              |              |              |          |           |       |        |
| Pd                                                                                | 16.74        | 362          |              | 26.5     | 27.7      | 28.8  | 30.0   |
| PdCl <sub>2</sub>                                                                 | 40.1         |              |              |          |           |       |        |
| PdO                                                                               |              |              |              | 37.6     | 49.5      | 61.3  |        |
| Phosphorus                                                                        |              |              |              |          |           |       |        |
| P                                                                                 |              | 0.66         | 12.4         | 14.2     |           |       |        |
| P <sub>4</sub> , $\Delta H_t = 0.521^{-77.8}$                                     | 0.659        | 56.5         | 58.9         | 73.3(g)  | 78.4      | 80.4  | 81.4   |
| PBr <sub>3</sub>                                                                  |              | 38.8         |              | 78.9     | 81.2      | 82.0  | 82.4   |
| PClF <sub>2</sub>                                                                 |              | 17.6         |              |          |           |       |        |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                        | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |           |          |          |
|--------------------------------------------------|--------------|--------------|--------------|----------|-----------|----------|----------|
|                                                  |              |              |              | 400 K    | 600 K     | 800 K    | 1000 K   |
| PClF <sub>3</sub>                                |              | 17.6         |              |          |           |          |          |
| PCl <sub>2</sub> F                               |              | 24.9         |              |          |           |          |          |
| PCl <sub>3</sub>                                 | 7.10         | 30.5         | 32.1         | 76.0(g)  | 79.7      | 81.2     | 81.9     |
| PCl <sub>5</sub>                                 |              |              | 64.9         | 120.1(g) | 126.8     | 129.5    | 130.7    |
| PF <sub>3</sub>                                  |              | 16.5         |              | 66.3(g)  | 74.0      | 77.6     | 79.5     |
| PF <sub>5</sub>                                  |              | 17.2         |              | 99.2(g)  | 114.7     | 121.9    | 125.6    |
| PH <sub>3</sub>                                  | 1.130        | 14.60        |              | 41.8     | 50.9      | 58.5     | 64.3     |
| P <sub>2</sub> H <sub>4</sub>                    |              | 28.8         |              |          |           |          |          |
| PI <sub>3</sub>                                  |              | 43.9         |              |          |           |          |          |
| P <sub>4</sub> O <sub>6</sub>                    | 14.06        | 43.43        |              | 172.1    | 200.8     | 213.5    | 220.0    |
| P <sub>4</sub> O <sub>10</sub>                   | 27.2         |              | 106.0        | 260.3    | 336.0(c)  |          |          |
| POBr <sub>3</sub>                                | 38           |              |              |          |           |          |          |
| POCl <sub>3</sub>                                | 13.1         | 34.3         | 38.6         | 92.0(g)  | 99.1      | 102.5    | 108.5    |
| POClF <sub>2</sub>                               |              | 25.4         |              | 79.3     | 91.6      | 97.7     | 101.1    |
| POCl <sub>2</sub> F                              |              | 30.96        |              | 87.7     | 96.6      | 100.9    | 103.2    |
| POF <sub>3</sub>                                 | 15.06        | 23.22        | 21.1         | 79.1     | 91.2      | 97.4     | 100.9    |
| PSCl <sub>3</sub>                                |              |              |              | 96.5     | 102.4     | 104.8    | 105.9    |
| PSF <sub>3</sub>                                 |              | 19.58        |              | 84.5     | 95.3      | 100.3    | 102.9    |
| P <sub>4</sub> S <sub>3</sub>                    | 9.2          | 59.8         |              | 184.1    | 184.1(lq) | 155.0(g) | 155.0    |
| Platinum                                         |              |              |              |          |           |          |          |
| Pt                                               | 22.17        | 469          | 545          | 26.4     | 27.5      | 28.5     | 29.6     |
| PtS                                              |              |              |              | 51.4     | 53.8      | 56.2     | 58.6     |
| PtS <sub>2</sub>                                 |              |              |              | 69.9     | 75.9      | 81.9     | 87.9     |
| Plutonium                                        |              |              |              |          |           |          |          |
| Pu, $\Delta H_t = 13.4^{122}$                    | 2.82         | 333.5        |              | 39.5     | 46.9      | 40.6     | 40.6     |
| $\Delta H_t = 2.9^{206}$                         |              |              |              |          |           |          |          |
| $\Delta H_t = 3.3^{319}$                         |              |              |              |          |           |          |          |
| $\Delta H_t = 66.9^{480}$                        |              |              |              |          |           |          |          |
| PuBr <sub>3</sub>                                | 55.2         | 236.4        | 292.5        |          |           |          |          |
| PuCl <sub>3</sub>                                | 63.6         | 241.0        | 304.6        |          |           |          |          |
| PuF <sub>3</sub>                                 | 59.8         |              | 374.9        |          |           |          |          |
| PuF <sub>4</sub>                                 | 65.3         |              | 299.6        |          |           |          |          |
| PuF <sub>6</sub>                                 | 17.6         | 29.9         | 48.5         |          |           |          |          |
| PuI <sub>3</sub>                                 | 50.2         |              |              |          |           |          |          |
| PuO <sub>2</sub>                                 |              | 559.8        |              |          |           |          |          |
| Polonium                                         |              |              |              |          |           |          |          |
| Po                                               |              | 102.91       |              |          |           |          |          |
| Potassium                                        |              |              |              |          |           |          |          |
| K                                                | 2.321        | 76.90        | 88.8         | 31.5(lq) | 30.1      | 29.8     | 30.7     |
| KAlCl <sub>4</sub>                               |              |              |              | 165.5    | 183.2     | 196.6    | 202.1    |
| K <sub>3</sub> AlCl <sub>6</sub>                 |              |              |              | 259.2    | 279.5     | 295.8    |          |
| K <sub>3</sub> AlF <sub>6</sub>                  |              |              |              | 244.5    | 269.4     | 286.8    | 302.0    |
| KBF <sub>4</sub> , $\Delta H_t = 14.06^{283}$    | 17.7         |              |              | 130.8    | 142.1     | 150.9    | 167.2    |
| KBH <sub>4</sub>                                 |              |              |              | 100.9    | 106.0     | 118.4    |          |
| KBO <sub>2</sub>                                 | 31           | 238.9        |              | 76.7     | 89.8      | 98.5     |          |
| K <sub>2</sub> B <sub>4</sub> O <sub>7</sub>     | 104          |              |              | 206.3    | 250.5     | 271.1    | 283.3    |
| KBr                                              | 25.5         | 149.2        |              | 53.8     | 56.4      | 60.4     | 68.0     |
| KCl                                              | 26.53        | 124.3        |              | 53.0     | 55.9      | 59.2     | 64.0     |
| KClO <sub>4</sub> , $\Delta H_t = 13.77^{299.6}$ |              |              |              | 138.5    | 165.3     |          |          |
| KCN, $\Delta H_t = 1.167^{-104.9}$               | 14.6         | 157.1        |              | 66.3     | 66.4      | 66.5(c)  | 66.5(lq) |



**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                  | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$   |           |          |          |
|------------------------------------------------------------|--------------|--------------|--------------|---------|-----------|----------|----------|
|                                                            |              |              |              | 400 K   | 600 K     | 800 K    | 1000 K   |
| K <sub>2</sub> CO <sub>3</sub>                             | 27.6         |              |              | 128.1   | 150.7     | 170.0    | 189.0    |
| K <sub>2</sub> CrO <sub>4</sub>                            | 29.0         |              |              |         |           |          |          |
| K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>              | 36.7         |              |              |         |           |          |          |
| KF                                                         | 27.2         | 141.8        | 231.8        | 51.0    | 54.3      | 57.4     | 61.2     |
| KH                                                         |              |              |              | 44.1    | 51.9      |          |          |
| KHF <sub>2</sub> , $\Delta H_t = 11.22^{196.7}$            | 6.62         |              |              | 86.1(c) | 104.6(lq) |          |          |
| KI                                                         | 24.0         | 190.9        | 202.4        | 53.9    | 57.3      | 62.6(c)  | 72.4(lq) |
| KNO <sub>3</sub> , $\Delta H_t = 5.10^{128}$               | 10.1         |              |              | 108.4   | 120.5     |          |          |
| K <sub>2</sub> O, $\Delta H_t = 6.20^{372}$                |              |              |              | 79.1    | 100.0     | 100.0    | 100.0    |
| KO <sub>2</sub> , $\Delta H_t = 0.302^{-79.7}$             |              |              |              | 83.9    | 90.2      |          |          |
| $\Delta H_t = 0.157^{-42.3}$                               |              |              |              |         |           |          |          |
| K <sub>2</sub> O <sub>2</sub>                              |              |              |              | 107     | 121       |          |          |
| KOH, $\Delta H_t = 6.4^{243}$                              | 8.60         | 142.7        | 192          | 72.5    | 79.0(c)   | 83.0(lq) | 83.0     |
| KPO <sub>3</sub>                                           | 8.8          |              |              |         |           |          |          |
| K <sub>3</sub> PO <sub>4</sub>                             | 37.2         |              |              |         |           |          |          |
| K <sub>2</sub> P <sub>2</sub> O <sub>7</sub>               | 58.6         |              |              |         |           |          |          |
| KReO <sub>4</sub>                                          | 85.4         |              |              |         |           |          |          |
| K <sub>2</sub> S                                           | 16.15        | 77.3         | 82.5         | 87.7    |           |          |          |
| K <sub>2</sub> SiO <sub>3</sub>                            | 50           |              |              | 135.6   | 157.7     | 170.7    | 179.1    |
| K <sub>2</sub> SO <sub>4</sub> , $\Delta H_t = 8.45^{584}$ | 34.39        |              |              | 147.6   | 172.5     | 199.6    | 226.1    |
| K <sub>2</sub> WO <sub>4</sub>                             | 19.5         |              |              |         |           |          |          |
| K <sub>2</sub> ZrCl <sub>6</sub>                           | 23.0         |              |              |         |           |          |          |
| Praseodymium                                               |              |              |              |         |           |          |          |
| Pr                                                         | 6.89         | 331          | 356          |         |           |          |          |
| Promethium                                                 |              |              |              |         |           |          |          |
| Pm                                                         | 7.13         | 289          | 328          |         |           |          |          |
| Protactinium                                               |              |              |              |         |           |          |          |
| Pa                                                         | 12.34        | 481          |              |         |           |          |          |
| PaCl <sub>3</sub>                                          | 92.9         | 61.3         |              |         |           |          |          |
| Radium                                                     |              |              |              |         |           |          |          |
| Ra                                                         | 8.5          | 113          |              |         |           |          |          |
| Radon                                                      |              |              |              |         |           |          |          |
| Rn                                                         | 3.247        | 18.10        |              |         |           |          |          |
| Rhenium                                                    |              |              |              |         |           |          |          |
| Re                                                         | 60.43        | 704          | 779          | 26.0    | 26.9      | 28.0     | 29.1     |
| ReF <sub>5</sub>                                           |              | 58.1         |              |         |           |          |          |
| ReF <sub>6</sub>                                           | 4.6          | 28.7         |              |         |           |          |          |
| ReF <sub>7</sub>                                           | 7.5          | 38.3         |              |         |           |          |          |
| ReO <sub>2</sub>                                           |              |              | 274.6        |         |           |          |          |
| ReO <sub>3</sub>                                           | 21.8         |              | 208.4        |         |           |          |          |
| Re <sub>2</sub> O <sub>7</sub>                             | 64.2         | 74.1         |              |         |           |          |          |
| ReOCl <sub>4</sub>                                         |              | 45.6         |              |         |           |          |          |
| ReOF <sub>4</sub>                                          | 13.5         | 61.0         |              |         |           |          |          |
| ReOF <sub>5</sub>                                          |              | 32.0         | 37.4         |         |           |          |          |
| Rhodium                                                    |              |              |              |         |           |          |          |
| Rh                                                         | 26.59        | 494          | 556          | 26.0    | 28.0      | 30.0     | 32.0     |
| Rh <sub>2</sub> O <sub>3</sub>                             |              |              |              | 109.9   | 121.4     | 133.0    | 144.5    |
| Rubidium                                                   |              |              |              |         |           |          |          |
| Rb                                                         | 2.19         | 75.77        |              | 31.7    | 30.9      | 30.7     |          |
| RbBr                                                       | 15.5         | 154.8        |              | 52.8    | 54.9      | 57.1(c)  | 66.9(lq) |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                  | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$     |          |         |          |
|------------------------------------------------------------|--------------|--------------|--------------|-----------|----------|---------|----------|
|                                                            |              |              |              | 400 K     | 600 K    | 800 K   | 1000 K   |
| RbCl                                                       | 18.4         | 165.7        |              | 52.3      | 54.3     | 56.4(c) | 64.0(lq) |
| RbClO <sub>4</sub> , $\Delta H_t = 12.59^{284}$            |              |              |              |           |          |         |          |
| RbF                                                        | 17.3         | 177.8        |              | 51.9      | 57.9     | 64.9    | 72.3     |
| RbI                                                        | 12.5         | 150.6        |              |           | 55.1     | 57.3(c) | 66.9(lq) |
| RbNO <sub>3</sub>                                          | 5.61         |              |              |           |          |         |          |
| RbOH                                                       | 6.78         |              |              |           |          |         |          |
| Ruthenium                                                  |              |              |              |           |          |         |          |
| Run, $\Delta H_t = 0.13^{1035}$                            | 38.59        | 591.6        |              | 24.5      | 25.7     | 27.0    | 28.2     |
| $\Delta H_t = 0.96^{1500}$                                 |              |              |              |           |          |         |          |
| Samarium                                                   |              |              |              |           |          |         |          |
| Sm, $\Delta H_t = 3.11^{917}$                              | 8.62         | 165          | 207          | 33.3      | 39.1     | 44.3    | 49.3     |
| Sm <sub>2</sub> O <sub>3</sub> , $\Delta H_t = 1.05^{922}$ |              |              |              | 125.2     | 135.3    | 141.4   | 146.3    |
| Scandium                                                   |              |              |              |           |          |         |          |
| Sc                                                         | 14.1         | 332.7        | 376          |           |          |         |          |
| ScCl <sub>3</sub>                                          |              |              |              | 96.7      | 102.7    | 108.7   | 114.6    |
| Sc <sub>2</sub> O <sub>3</sub>                             |              |              |              | 106.4     | 111.1    | 115.8   | 120.5    |
| Selenium                                                   |              |              |              |           |          |         |          |
| Se, $\Delta H_t = 0.75^{150}$                              | 6.69         | 95.48        |              | 28.1(c)   | 35.2(lq) | 35.1    |          |
| SeF <sub>4</sub>                                           |              | 47.2         |              |           |          |         |          |
| SeF <sub>6</sub>                                           | 8.4          |              | 26.8         | 127.9     | 141.3    | 147.1   | 150.7    |
| SeO <sub>2</sub>                                           |              | 94.5         |              |           |          |         |          |
| SeOCl <sub>2</sub>                                         | 4.23         | 42.7         |              |           |          |         |          |
| Silicon                                                    |              |              |              |           |          |         |          |
| Si                                                         | 50.21        | 359          | 450          | 22.3      | 24.5     | 25.7    | 26.5     |
| SiBr <sub>4</sub>                                          |              | 37.9         |              | 146.4(lq) | 104.9(g) | 106.2   | 106.2    |
| SiC beta                                                   |              |              |              | 34.1      | 41.8     | 45.9    | 48.4     |
| SiCl <sub>4</sub>                                          | 7.60         | 28.7         | 29.7         | 96.9(g)   | 102.6    | 104.8   | 106.0    |
| SiClF <sub>3</sub>                                         |              | 18.7         |              | 88.3      | 97.5     | 101.7   | 103.8    |
| SiCl <sub>2</sub> F <sub>2</sub>                           |              | 21.2         |              |           |          |         |          |
| SiF <sub>4</sub>                                           |              |              | 25.7         | 83.1      | 94.1     | 99.4    | 102.3    |
| SiH <sub>4</sub>                                           | 0.67         | 12.1         |              | 51.5      | 65.9     | 76.7    | 84.5     |
| Si <sub>2</sub> H <sub>6</sub>                             |              | 21.2         |              |           |          |         |          |
| Si <sub>3</sub> H <sub>8</sub>                             |              | 28.5         |              |           |          |         |          |
| SiH <sub>3</sub> Br                                        |              | 24.4         |              |           |          |         |          |
| SiH <sub>2</sub> Br <sub>2</sub>                           |              | 31           |              |           |          |         |          |
| SiHBr <sub>3</sub>                                         |              | 34.8         |              |           |          |         |          |
| SiH <sub>3</sub> Cl                                        |              | 21           |              | 60.7      | 74.0     | 83.1    | 89.4     |
| SiH <sub>2</sub> Cl <sub>2</sub>                           |              | 25.2         | 24.2         | 71.5      | 82.9     | 90.0    | 94.6     |
| SiHCl <sub>3</sub>                                         |              | 26.6         | 25.7         | 83.7      | 92.5     | 97.2    | 100.2    |
| SiH <sub>3</sub> F                                         |              | 18.8         |              | 57.2      | 71.8     | 81.7    | 88.3     |
| SiH <sub>2</sub> F <sub>2</sub>                            |              | 16.3         |              |           |          |         |          |
| SiHF <sub>3</sub>                                          |              | 16.2         |              |           |          |         |          |
| SiI <sub>4</sub>                                           | 19.7         | 56.9         | 79           | 164.0(lq) | 106.0(g) | 106.9   | 107.3    |
| Si <sub>3</sub> N <sub>4</sub>                             |              |              |              | 110.7     | 129.7    | 145.8   | 158.2    |
| SiO <sub>2</sub> cristobalite                              | 8.51         |              |              |           |          |         |          |
| SiO <sub>2</sub> quartz                                    | 7.7          |              | 600          | 53.5      | 64.4     | 76.2    | 68.94    |
| $\Delta H_t = 0.73^{574}$                                  |              |              |              |           |          |         |          |
| $\Delta H_t = 2.0^{806}$                                   |              |              |              |           |          |         |          |
| SiOF <sub>2</sub>                                          |              |              |              | 61.3      | 70.4     | 75.0    | 77.6     |
| SiS <sub>2</sub>                                           | 20.9         |              |              | 78.6      | 81.7     | 83.4    | 85.4     |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                  | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$    |          |           |           |
|----------------------------------------------------------------------------|--------------|--------------|--------------|----------|----------|-----------|-----------|
|                                                                            |              |              |              | 400 K    | 600 K    | 800 K     | 1000 K    |
| Silver                                                                     |              |              |              |          |          |           |           |
| Ag                                                                         | 11.95        | 258          |              | 25.7     | 26.8     | 28.4      | 30.0      |
| AgBr                                                                       | 9.12         | 198          |              | 59.0     | 71.8(c)  | 62.3(lq)  | 62.3      |
| AgCl                                                                       | 13.2         | 199          |              | 56.9     | 54.4     | 54.4      | 54.4      |
| Ag <sub>2</sub> CO <sub>3</sub>                                            |              |              |              |          | 122.6    |           |           |
| AgF                                                                        | 16.7         | 179.1        |              | 54.1(c)  | 58.4     |           |           |
| AgI, $\Delta H_t = 6.15^{147}$                                             | 9.41         | 143.9        |              | 64.7     | 56.5     | 56.5      | 58.6(lq)  |
| AgNO <sub>3</sub> , $\Delta H_t = 2.5^{160}$                               | 11.5         |              |              | 112.5    | 128.0    |           |           |
| Ag <sub>2</sub> O                                                          |              |              |              | 73.0     |          |           |           |
| Ag <sub>2</sub> S, $\Delta H_t = 5.86^{176}$                               | 14.1         |              |              | 86.6     | 90.5     | 90.5      | 90.5      |
| $\Delta H_t = 5.86^{586}$                                                  |              |              |              |          |          |           |           |
| Sodium                                                                     |              |              |              |          |          |           |           |
| Na                                                                         | 2.60         | 97.42        | 107.5        | 31.5(lq) | 29.3     | 29.9      | 29.0      |
| NaAlCl <sub>4</sub>                                                        |              |              |              | 164.8(c) |          |           |           |
| Na <sub>3</sub> AlCl <sub>6</sub>                                          |              |              |              | 254.4    | 273.0    |           |           |
| Na <sub>3</sub> AlF <sub>6</sub> , $\Delta H_t = 8.37^{565}$               | 107.28       |              |              | 234.6    | 261.8    | 196.8     | 282.8     |
| $\Delta H_t = 0.42^{880}$                                                  |              |              |              |          |          |           |           |
| NaAlO <sub>2</sub> , $\Delta H_t = 1.297^{467}$                            |              |              |              | 83.4     | 94.3     | 98.7      | 102.3     |
| NaBH <sub>4</sub> , $\Delta H_t = 0.999^{-83.3}$                           |              |              |              | 94.6     | 108.6    |           |           |
| NaBO <sub>2</sub>                                                          | 36.2         | 239.7        | 322.2        | 75.4     | 88.6     | 97.2      | 103.2     |
| Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                              | 76.9         |              |              | 221.7    | 268.6    | 444.9(lq) |           |
| NaBr                                                                       | 26.11        | 160.7        | 217.5        | 53.5     | 56.1     | 58.6      | 61.1      |
| NaBrO <sub>3</sub>                                                         | 28.11        |              |              |          |          |           |           |
| NaCl                                                                       | 28.16        |              |              | 52.3     | 55.5     | 59.3      | 72.5      |
| NaClO <sub>3</sub>                                                         | 22.1         |              |              |          |          |           |           |
| NaClO <sub>4</sub> , $\Delta H_t = 13.98^{308}$                            |              |              |              | 136.0(c) |          |           |           |
| NaCN                                                                       | 8.79         | 148.1        | 172.8        | 68.7     | 68.8     | 69.0      |           |
| Na <sub>2</sub> CO <sub>3</sub> , $\Delta H_t = 0.690^{450}$               | 29.64        |              |              | 125.1    | 163.3    | 153.3     | 179.8     |
| NaF                                                                        | 33.35        | 176.1        | 284.9        | 49.6     | 52.7     | 55.7      | 59.5      |
| NaH                                                                        |              |              |              | 42.5     | 50.7     |           |           |
| NaI                                                                        | 23.60        |              |              | 53.8     | 56.2     | 58.5(c)   | 64.9(lq)  |
| NaIO <sub>3</sub> , $\Delta H_t = 35.1^{422}$                              |              |              |              |          |          |           |           |
| NaNO <sub>3</sub>                                                          | 15           |              |              |          |          |           |           |
| NaO <sub>2</sub> , $\Delta H_t = 1.464^{-76.7}$                            |              |              |              | 76.3     | 84.5     | 92.6      |           |
| $\Delta H_t = 1.548^{-49.9}$                                               |              |              |              |          |          |           |           |
| Na <sub>2</sub> O, $\Delta H_t = 1.76^{750.1}$                             | 47.7         |              |              | 75.8     | 85.7     | 91.3      | 94.9      |
| $\Delta H_t = 11.92^{970.1}$                                               |              |              |              |          |          |           |           |
| Na <sub>2</sub> O <sub>2</sub> , $\Delta H_t = 5.73^{512}$                 |              |              |              | 97.7     | 108.4    | 113.6     |           |
| NaOH, $\Delta H_t = 72^{299.6}$                                            | 6.60         | 175.3        | 228.2        | 64.9(c)  | 86.1(lq) | 84.9      | 83.7      |
| Na <sub>2</sub> S                                                          | 19.3         |              |              | 20.1     | 20.9     | 21.5      | 22.0      |
| Na <sub>2</sub> S <sub>2</sub>                                             |              |              |              | 104.3    | 115.4(c) | 124.7(lq) | 124.7     |
| Na <sub>2</sub> SiO <sub>3</sub>                                           | 51.8         |              |              | 127.8    | 147.1    | 159.7     | 169.4     |
| Na <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> , $\Delta H_t = 0.42^{678}$ | 35.6         |              |              | 183.4    | 217.6    | 235.2     | 292.9     |
| Na <sub>2</sub> SO <sub>4</sub> , $\Delta H_t = 10.91^{241}$               | 23.6         |              |              | 145.1    | 175.3    | 187.3     | 200.3     |
| Na <sub>2</sub> TiO <sub>3</sub>                                           | 70.3         |              |              |          |          |           |           |
| Na <sub>2</sub> WO <sub>4</sub> , $\Delta H_t = 30.85^{587.7}$             | 23.80        |              |              | 155.3    | 178.2    | 198.7     |           |
| $\Delta H_t = 4.113^{588.9}$                                               |              |              |              |          |          |           |           |
| Strontium                                                                  |              |              |              |          |          |           |           |
| Sr, $\Delta H_t = 0.84^{547}$                                              | 7.43         | 136.9        | 164.0        | 27.8     | 29.8     | 31.9      | 34.1      |
| SrBr <sub>2</sub> , $\Delta H_t = 12.2^{645}$                              | 10.1         | 194.1        | 310          | 79.0     | 82.7     | 87.6(c)   | 116.4(lq) |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                                 | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$     |           |           |           |
|---------------------------------------------------------------------------|--------------|--------------|--------------|-----------|-----------|-----------|-----------|
|                                                                           |              |              |              | 400 K     | 600 K     | 800 K     | 1000 K    |
| $\text{SrCl}_2$ , $\Delta H_t = 6.0^{727}$                                | 17.5         | 248.1        | 356          | 78.9      | 83.7      | 90.8      | 105.8     |
| $\text{SrCO}_3$ , $\Delta H_t = 19.7^{924}$                               | 40           |              |              | 95.1      | 107.1     | 116.1     | 124.0     |
| $\text{SrF}_2$ , $\Delta H_t = 0.04^{1148}$<br>$\Delta H_t = 0.04^{1211}$ | 28.5         | 320          | 451.0        | 74.7      | 79.8      | 81.0      | 85.8      |
| $\text{SrI}_2$                                                            | 19.67        | 189.7        | 286.6        | 80.7      | 86.3      | 91.8(c)   | 110.0(lq) |
| $\text{SrH}_2$                                                            | 23           |              |              |           |           |           |           |
| $\text{SrMoO}_4$                                                          |              |              |              | 131.5     | 145.4     | 154.0     | 161.2     |
| $\text{SrO}$                                                              | 81           |              |              | 48.5      | 52.0      | 54.3      | 56.1      |
| $\text{SrO}_2$                                                            |              |              |              | 81.3      | 85.0      |           |           |
| $\text{Sr(OH)}_2$                                                         | 23           |              |              | 88.5      | 115.0(c)  | 157.8(lq) | 157.8     |
| $\text{SrS}$                                                              | 63           |              |              | 50.2      | 53.2      | 54.9      | 56.2      |
| $\text{SrSO}_4$                                                           | 36           |              |              | 113.5     | 124.6     | 135.7     | 146.9     |
| Sulfur                                                                    |              |              |              |           |           |           |           |
| S monoclinic<br>$\Delta H_t = 0.400^{95.2}$                               | 1.727        | 45           | 62.2         | 23.2      | 23.3(lq)  | 21.8(g)   | 21.5      |
| $\text{S}_8$                                                              |              |              |              | 167.1     | 177.9     | 186.7     | 193.6     |
| $\text{SCl}_2$                                                            |              | 32.4         |              | 53.6      | 56.0      | 56.9      | 57.4      |
| $\text{S}_2\text{Cl}_2$                                                   |              | 36.0         |              | 124.3(lq) | 80.8(g)   | 82.6      | 83.5      |
| $\text{SF}_4$                                                             |              | 26.4         |              | 87.5      | 97.3      | 101.7     | 103.8     |
| $\text{SF}_6$                                                             | 5.02         | 17.1         | 9.0          | 116.4     | 136.1     | 144.8     | 149.3     |
| $\text{S}_2\text{F}_{10}$                                                 |              |              |              | 211.4     | 246.4     | 261.8     | 269.2     |
| $\text{SO}_2$                                                             | 7.40         | 24.94        | 22.92        | 43.43     | 48.9      | 52.3      | 54.3      |
| $\text{SO}_3$                                                             | 8.60         | 40.7         | 43.14        | 57.7      | 67.3      | 72.8      | 76.0      |
| $\text{SOCl}_2$                                                           |              | 31.7         | 31           | 71.3      | 76.4      | 78.9      | 80.3      |
| $\text{SOF}_2$                                                            |              | 21.8         |              | 64.3      | 72.4      | 76.4      | 78.6      |
| $\text{SO}_2\text{Cl}_2$                                                  |              | 31.38        | 30.1         | 85.2      | 94.5      | 99.4      | 102.1     |
| $\text{SO}_2\text{ClF}$                                                   |              |              |              | 81.1      | 92.1      | 97.9      | 101.1     |
| $\text{SO}_2\text{F}_2$                                                   |              | 20.0         |              | 76.5      | 89.3      | 96.1      | 99.9      |
| Tantalum                                                                  |              |              |              |           |           |           |           |
| Ta                                                                        | 36.57        | 732.8        | 778          | 25.8      | 26.8      | 27.5      | 27.9      |
| $\text{TaB}_2$                                                            | 83.7         |              |              | 57.6      | 66.6      | 72.2      | 83.3      |
| $\text{TaBr}_5$                                                           | 45.6         | 62.3         |              | 168.2     |           |           |           |
| TaC                                                                       | 105          |              |              | 41.7      | 46.5      | 49.1      | 51.1      |
| $\text{Ta}_2\text{C}$                                                     |              |              |              | 66.7      | 72.4      | 76.2      | 79.5      |
| $\text{TaCl}_5$                                                           | 41.6         | 54.8         | 94.1         | 148.(c)   | 129.(g)   | 131       | 132       |
| $\text{TaF}_5$                                                            | 18.8         | 56.9         |              | 182.0(lq) |           |           |           |
| $\text{TaI}_5$                                                            | 41.8         | 64.9         |              | 164.6     | 182.0(c)  | 120.0(g)  | 120.6     |
| TaN                                                                       | 67           |              |              | 45.4      | 51.9      | 58.5      | 65.0      |
| $\text{TaO}_2$                                                            |              |              |              | 47.7      | 52.3      | 54.6      | 55.7      |
| $\text{Ta}_2\text{O}_5$                                                   | 120          |              |              | 147.5     | 164.4     | 175.2     | 182.8     |
| Technetium                                                                |              |              |              |           |           |           |           |
| Tc                                                                        | 33.29        | 585.2        |              | 25.1      | 26.8      | 28.5      | 30.1      |
| $\text{TcF}_6$                                                            | 4.72         | 31.1         |              |           |           |           |           |
| $\text{TcO}_3\text{F}$                                                    | 22.5         | 39.5         |              |           |           |           |           |
| Tellurium                                                                 |              |              |              |           |           |           |           |
| Te                                                                        | 17.49        | 114.1        |              | 28.0      | 32.3(c)   | 37.7(lq)  | 37.7      |
| $\text{TeCl}_4$                                                           | 18.8         | 77           |              | 138.9(c)  | 222.6(lq) | 108.8(g)  | 108.8     |
| $\text{TeF}_4$                                                            |              | 34.3         |              |           |           |           |           |
| $\text{TeF}_6$                                                            |              |              | 28.2         | 132.2     | 143.8     | 148.7     | 151.7     |
| $\text{Te}_2\text{F}_{10}$                                                |              | 39.5         |              |           |           |           |           |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                    | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$     |          |          |        |
|----------------------------------------------|--------------|--------------|--------------|-----------|----------|----------|--------|
|                                              |              |              |              | 400 K     | 600 K    | 800 K    | 1000 K |
| TeH <sub>2</sub>                             |              | 23.9         |              |           |          |          |        |
| TeO <sub>2</sub>                             | 29.1         |              |              | 67.9      | 72.5     | 76.1     | 79.2   |
| Terbium                                      |              |              |              |           |          |          |        |
| Tb                                           | 10.15        | 293          | 389          |           |          |          |        |
| Thallium                                     |              |              |              |           |          |          |        |
| Tl, $\Delta H_t = 0.38^{234}$                | 4.14         | 165          | 181          | 27.5(c)   | 30.1(lq) | 30.1     | 30.1   |
| TlBr                                         | 16.4         | 99.6         |              | 53.5      | 59.5(c)  | 75.5(lq) | 67.8   |
| TlCl                                         | 15.56        | 102.2        |              | 53.6      | 55.2(c)  | 59.4(lq) | 59.4   |
| Tl <sub>2</sub> CO <sub>3</sub>              | 18.4         |              |              |           |          |          |        |
| TlF                                          | 13.87        | 115.9        |              |           | 66.8(lq) | 67.3     |        |
| TlI                                          | 14.73        | 104.7        |              | 53.9      | 60.6(c)  | 72.0(lq) | 72.0   |
| TlNO <sub>3</sub>                            | 9.56         |              |              |           |          |          |        |
| Tl <sub>2</sub> O                            | 30.3         |              |              |           |          |          |        |
| Tl <sub>2</sub> O <sub>3</sub>               | 53           |              |              |           |          |          |        |
| Tl <sub>2</sub> S                            | 12           | 154          |              |           |          |          |        |
| Tl <sub>2</sub> SO <sub>4</sub>              | 23.0         |              |              |           |          |          |        |
| Thorium                                      |              |              |              |           |          |          |        |
| Th, $\Delta H_t = 2.73^{1360}$               | 13.81        | 514          |              | 28.4      | 30.5     | 32.7     | 34.4   |
| ThBr <sub>4</sub>                            | 66.9         |              |              |           |          |          |        |
| ThCl <sub>4</sub> , $\Delta H_t = 5.0^{406}$ | 40.2         | 146.4        |              | 126.7     | 132.7    | 136.4    | 139.6  |
| ThF <sub>4</sub>                             | 44.0         | 258          |              |           |          |          |        |
| ThI <sub>4</sub>                             | 61.4         | 56.9         |              |           |          |          |        |
| Th <sub>3</sub> N <sub>4</sub>               |              |              |              | 169.5     | 196.5    | 222.7    |        |
| ThO <sub>2</sub>                             | 1218.0       |              |              | 67.4      | 72.4     | 75.3     | 77.7   |
| ThOCl <sub>2</sub>                           |              |              |              | 97.0      | 102.5    | 105.9    | 108.6  |
| Th(SO <sub>4</sub> ) <sub>2</sub>            |              |              |              | 197.0     | 243.2    | 289.4    |        |
| Thullium                                     |              |              |              |           |          |          |        |
| Tm                                           | 16.84        | 247          | 232.2        |           |          |          |        |
| Tin                                          |              |              |              |           |          |          |        |
| Sn white, $\Delta H_t = 2.09^{13}$           | 7.03         | 296.1        |              | 28.9      | 28.9(c)  | 28.7(lq) | 28.7   |
| SnBr <sub>2</sub>                            | 7.2          | 102          |              |           |          |          |        |
| SnBr <sub>4</sub>                            | 11.9         | 43.5         |              | 158.0(lq) | 106.8(g) | 107.3    | 107.5  |
| SnCl <sub>2</sub>                            | 12.8         | 86.8         |              | 83.3(c)   | 92.1(lq) | 92.1     | 92.1   |
| SnCl <sub>4</sub>                            | 9.20         | 34.9         |              |           |          |          |        |
| SnH <sub>4</sub>                             |              | 19.1         |              |           |          |          |        |
| SnI <sub>2</sub>                             |              | 105          |              |           |          |          |        |
| SnO                                          |              |              |              | 45.8      | 48.7     | 51.7     | 54.6   |
| SnO <sub>2</sub> , $\Delta H_t = 1.88^{410}$ |              |              |              | 64.4      | 73.9     | 78.5     | 81.8   |
| $\Delta H_t = 1.26^{540}$                    |              |              |              |           |          |          |        |
| SnS, $\Delta H_t = 0.67^{602}$               |              |              |              | 50.5      | 55.5     | 61.3     |        |
| SnS <sub>2</sub>                             |              |              |              | 71.9      | 75.4     | 79.0     | 82.5   |
| Titanium                                     |              |              |              |           |          |          |        |
| Ti, $\Delta H_t = 4.2^{893}$                 | 14.15        | 425          | 469          | 26.9      | 28.6     | 29.5     | 32.1   |
| TiB                                          |              |              |              | 40.3      | 48.6     | 50.9     | 51.9   |
| TiB <sub>2</sub>                             | 100.4        |              |              | 54.9      | 66.2     | 72.1     | 76.9   |
| TiBr <sub>2</sub>                            |              |              | 206.2        | 79.9      | 82.1     | 84.4     | 86.7   |
| TiBr <sub>3</sub>                            |              |              | 138.8        | 105.8     | 125.5    | 147.3    | 156.7  |
| TiBr <sub>4</sub>                            | 12.9         | 44.4         |              | 151.9(lq) | 106.1(g) | 106.9    | 107.3  |
| TiC                                          | 71           |              |              | 40.7      | 47.7     | 49.9     | 51.2   |
| TiCl <sub>2</sub>                            |              | 232          | 212          | 73.4      | 78.4     | 82.2     | 85.9   |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                   | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$     |           |           |          |
|-------------------------------------------------------------|--------------|--------------|--------------|-----------|-----------|-----------|----------|
|                                                             |              |              |              | 400 K     | 600 K     | 800 K     | 1000 K   |
| TiCl <sub>3</sub>                                           |              | 124          | 166.3        | 98.6      | 102.0     | 104.4     | 106.7    |
| TiCl <sub>4</sub>                                           | 9.97         | 36.2         |              | 146.2(lq) | 104.4(g)  | 106.0     | 106.7    |
| TiF <sub>3</sub>                                            |              |              | 222          | 93        | 98        | 103       | 109      |
| TiF <sub>4</sub>                                            |              |              | 97.9         | 126.7(c)  | 100.2(g)  | 103.3     | 104.9    |
| TiH <sub>2</sub>                                            |              |              |              | 39.3      | 53.8      | 63.1      | 68.5     |
| TiI <sub>2</sub>                                            |              |              | 217          | 87.0      | 88.4      | 89.9      | 91.3     |
| TiI <sub>3</sub>                                            |              |              |              | 117.5     | 119.0     | 120.4(c)  | 20.6(g)  |
| TiI <sub>4</sub> , $\Delta H_t = 9.9^{106}$                 | 19.8         | 58.4         |              | 148.1(c)  | 156.6(lq) | 25.7(g)   | 27.8     |
| TiN                                                         | 66.9         |              |              | 43.8      | 48.7      | 50.6      | 52.1     |
| TiO, $\Delta H_t = 4.2^{992}$                               | 41.8         |              |              | 45.0      | 50.8      | 55.2      | 59.1     |
| TiO <sub>2</sub> rutile                                     | 58.0         |              | 673          | 63.6      | 70.9      | 73.9      | 75.3     |
| Ti <sub>2</sub> O <sub>3</sub> , $\Delta H_t = 1.138^{197}$ | 105          |              |              | 117.5     | 136.4     | 143.0     | 146.4    |
| Tungsten                                                    |              |              |              |           |           |           |          |
| W                                                           | 52.31        | 806.7        | 851          | 24.9      | 25.9      | 26.7      | 27.6     |
| WBr <sub>5</sub>                                            | 17.1         | 81.5         |              | 166.(c)   | 182.(lq)  | 132.2(g)  | 132.5    |
| WBr <sub>6</sub>                                            |              |              |              | 192.5(c)  | 156.3(g)  | 157.0     | 157.4    |
| WCl <sub>4</sub>                                            |              |              |              | 135.3     | 146.2(c)  | 106.7(g)  | 107.2    |
| WCl <sub>5</sub>                                            | 20.5         | 68.1         | 100          | 167.4(c)  | 129.5(g)  | 131.0     | 131.8    |
| WCl <sub>6</sub> , $\Delta H_t = 4.1^{177}$                 | 6.60         | 52.7         | 79.2         | 192.5(c)  | 200.8(lq) | 155.8(g)  | 156.6    |
| W(CO) <sub>6</sub>                                          |              |              | 72.0         |           |           |           |          |
| WF <sub>6</sub> , $\Delta H_t = 2.067^{-8.5}$               | 4.10         | 27.05        | 26.65        | 132.4(g)  | 145.0     | 150.3     | 153.0    |
| WO <sub>2</sub>                                             |              |              | 666.3        | 63.4      | 71.3      | 75.5      | 78.2     |
| WO <sub>3</sub> , $\Delta H_t = 1.49^{777}$                 | 73.4         | 76.6         | 550.2        | 82.2      | 93.1      | 98.2      | 101.7    |
| WOCl <sub>4</sub>                                           | 45           | 67.8         |              | 157.(c)   | 123.2(g)  | 127.0     | 129.1    |
| WOF <sub>4</sub>                                            | 5.0          | 56           |              | 107.8     | 119.8     | 125.0     | 127.8    |
| WO <sub>2</sub> Cl <sub>2</sub>                             |              |              |              | 115.1     | 135.6(c)  |           |          |
| Uranium                                                     |              |              |              |           |           |           |          |
| U, $\Delta H_t = 2.93^{672}$<br>$\Delta H_t = 4.791^{772}$  | 9.14         | 417.1        | 525          | 29.0      | 34.8      | 41.6      | 41.8     |
| UBr <sub>3</sub>                                            | 43.9         |              |              |           |           |           |          |
| UBr <sub>4</sub>                                            | 55.2         | 119.2        |              | 131.4     | 140.1(c)  | 163.2(lq) | 163.2    |
| UC                                                          |              |              |              | 64.6      | 58.3      | 60.3      | 62.2     |
| UCl <sub>3</sub>                                            | 46.4         | 193.0        |              | 102.8     | 107.7     | 113.6     | 119.9    |
| UCl <sub>4</sub>                                            | 44.8         | 141.4        |              | 126.1     | 134.4     | 142.0     | 162.5    |
| UCl <sub>5</sub>                                            | 35.6         | 75.3         |              | 150.9     | 159.8(c)  | 186.7(lq) | 134.5(g) |
| UCl <sub>6</sub>                                            | 20.9         | 50.2         |              | 182.8     | 214.0     | 158.8     | 168.0    |
| UF <sub>3</sub>                                             |              |              |              | 99.0      | 104.9     | 111.0     | 117.2    |
| UF <sub>4</sub>                                             | 42.7         | 221.8        |              | 119.1     | 125.0     | 130.9     | 136.8    |
| UF <sub>5</sub>                                             | 33.5         |              |              | 136.4     | 143.1(c)  | 166.6(lq) |          |
| UF <sub>6</sub>                                             | 19.19        | 28.90        | 48.20        | 140.5(g)  | 148.7     | 152.2     | 154.4    |
| UH <sub>3</sub>                                             |              |              |              | 50.9      | 57.4      | 66.1      |          |
| UI <sub>4</sub>                                             | 70.7         | 130.6        |              | 140.6     | 149.5(c)  | 165.7(lq) | 165.7    |
| UN                                                          |              |              |              | 52.2      | 56.3      | 58.3      | 59.8     |
| UO <sub>2</sub>                                             |              |              |              | 72.7      | 79.8      | 83.2      | 85.5     |
| UO <sub>3</sub>                                             |              |              |              | 88.9      | 95.3      | 99.0      |          |
| U <sub>3</sub> O <sub>8</sub>                               |              |              |              | 266.0     | 290.7     | 304.2     |          |
| UOCl <sub>2</sub>                                           |              |              |              | 101.9     | 109.6     | 115.1     |          |
| UO <sub>2</sub> Cl <sub>2</sub>                             |              |              |              | 118.1     | 126.2     | 130.0     |          |
| UO <sub>2</sub> F <sub>2</sub>                              |              |              |              | 113.9     | 122.5     | 126.7     | 129.5    |

**TABLE 6.4** Heats of Fusion, Vaporization, and Sublimation and Specific Heat at Various Temperatures of the Elements and Inorganic Compounds (*Continued*)

| Substance                                                     | $\Delta H_m$ | $\Delta H_v$ | $\Delta H_s$ | $C_p$     |           |          |         |
|---------------------------------------------------------------|--------------|--------------|--------------|-----------|-----------|----------|---------|
|                                                               |              |              |              | 400 K     | 600 K     | 800 K    | 1000 K  |
| Vanadium                                                      |              |              |              |           |           |          |         |
| V                                                             | 21.5         | 459          | 516          | 26.2      | 27.5      | 28.7     | 30.1    |
| VCl <sub>4</sub>                                              | 2.30         | 41.4         | 42.5         | 161.7(lq) | 100.1(g)  | 102.6    | 104.7   |
| VF <sub>5</sub>                                               | 50.0         | 44.5         |              |           |           |          |         |
| VN, $\Delta H_{dec} = 227.6^{2346}$                           |              |              | 741          | 43.3      | 48.2      | 51.2     | 53.7    |
| VO                                                            | 63           |              |              | 49.6      | 53.5      | 57.1     | 60.5    |
| VO <sub>2</sub> , $\Delta H_t = 4.21^{72}$                    | 56.9         |              |              | 67.2      | 74.3      | 77.8     | 80.2    |
| V <sub>2</sub> O <sub>3</sub> , $\Delta H_t = 1.623^{-104.3}$ | 117.2        |              |              | 117.5     | 127.3     | 132.6    | 138.0   |
| V <sub>2</sub> O <sub>4</sub> , $\Delta H_t = 9.0^{67}$       | 112.1        |              |              | 135.3     | 148.4     | 155.5    | 160.7   |
| V <sub>2</sub> O <sub>5</sub>                                 | 64.5         | 263.6        |              | 151.0     | 168.3     | 177.3    | 183.7   |
| VOCl <sub>3</sub>                                             |              | 36.8         |              |           |           |          |         |
| Xenon                                                         |              |              |              |           |           |          |         |
| Xe                                                            | 1.81         | 12.64        |              | 20.79(g)  | 20.79     | 20.79    | 20.79   |
| Ytterbium                                                     |              |              |              |           |           |          |         |
| Yb                                                            | 7.66         | 159          |              |           |           |          |         |
| Yttrium                                                       |              |              |              |           |           |          |         |
| Y, $\Delta H_t = 4.97^{1485}$                                 | 11.42        | 365          | 425          | 27.3      | 28.5      | 29.9     | 31.5    |
| Y <sub>2</sub> O <sub>3</sub> , $\Delta H_t = 1.30^{1057}$    | 105          |              |              | 113.3     | 121.3     | 124.7    | 126.9   |
| Zinc                                                          |              |              |              |           |           |          |         |
| Zn                                                            | 7.32         | 123.6        |              | 26.3      | 28.6(c)   | 31.4(lq) | 31.4    |
| ZnBr <sub>2</sub>                                             | 16.7         | 118          |              | 70.1(c)   | 78.8(lq)  | 113.8    | 61.5(g) |
| ZnCl <sub>2</sub>                                             | 10.25        | 126          |              | 69.9(c)   | 100.8(lq) | 100.8    | 100.8   |
| ZnF <sub>2</sub>                                              |              | 190.1        |              | 66.9      | 69.1      | 71.4     | 73.7    |
| ZnO, $\Delta H_t = 13.4^{1020}$                               | 52.3         |              |              | 49.4      | 52.4      | 54.1     | 55.5    |
| Zn <sub>2</sub> SiO <sub>4</sub>                              |              |              |              | 129.4     | 141.4     | 153.4    | 165.4   |
| ZnSO <sub>4</sub> , $\Delta H_t = 20.3^{740}$                 |              |              |              | 116.0     | 137.4     | 139.7    | 142.0   |
| Zirconium                                                     |              |              |              |           |           |          |         |
| Zr, $\Delta H_t = 4.02^{862}$                                 | 21.00        | 573          | 610.0        | 25.9      | 27.3      | 29.0     | 31.1    |
| ZrB <sub>2</sub>                                              | 104.6        |              |              | 57.5      | 65.8      | 69.7     | 72.1    |
| ZrBr <sub>2</sub>                                             | 63           | 131.5        | 230          | 87.9      | 90.2      | 92.5     | 94.8    |
| ZrBr <sub>4</sub>                                             |              |              |              | 129.3     | 133.3(c)  | 107.2(g) | 107.6   |
| ZrC                                                           | 79.5         |              |              | 43.6      | 49.4      | 52.3     | 53.4    |
| ZrCl <sub>2</sub>                                             | 27           | 45.0         |              | 76.0      | 80.0      | 83.1     | 85.9    |
| ZrCl <sub>3</sub>                                             |              |              | 190          | 101       | 106       | 109      | 112     |
| ZrCl <sub>4</sub>                                             | 50           |              | 110.5        | 125.4     | 131.1(c)  | 106.5(g) | 107.1   |
| ZrF <sub>2</sub>                                              | 33           | 289          | 404          | 70        | 76        | 81       | 84      |
| ZrF <sub>4</sub>                                              | 64.2         |              | 237.7        | 113.5     | 124.0     | 129.4    | 134.1   |
| ZrI <sub>2</sub>                                              | 25.1         | 113          |              | 95.0      | 96.6      | 106.1    | 123.6   |
| ZrI <sub>3</sub>                                              |              |              | 176          | 105.9     | 106.7     | 107.1(c) | 82.9(g) |
| ZrI <sub>4</sub>                                              |              |              | 126.4        | 131.0     | 134.6(c)  | 107.6(g) | 107.6   |
| ZrN                                                           | 67.4         |              |              | 44.8      | 48.7      | 50.9     | 52.7    |
| ZrO <sub>2</sub> , $\Delta H_t = 5.02^{1205}$                 | 87.0         | 624          |              | 63.9      | 70.2      | 73.5     | 75.7    |
| ZrSiO <sub>4</sub>                                            |              |              |              | 114.6     | 133.7     | 142.7    | 147.3   |

6.2 CRITICAL PHENOMENA

The *critical temperature*,  $T_c$ , of a gas is the temperature above which the gas cannot be liquefied no matter how high the pressure.

The *critical pressure*,  $P_c$ , is the lowest pressure which will liquefy the gas at its critical temperature.

The *critical volume*,  $V_c$ , is the volume of 1 mol at the critical temperature and the critical pressure. It can be computed from the critical density,  $\rho_c$ , as follows:

$$\frac{\text{Molecular weight (in g} \cdot \text{mol}^{-1})}{\rho_c \text{ (in g} \cdot \text{cm}^{-3})} = V_c \text{ (in cm}^3 \cdot \text{mol}^{-1})$$

The critical pressure, critical molar volume, and critical temperature are the values of the pressure, molar volume, and thermodynamic temperature at which the densities of coexisting liquid and gaseous phases just become identical. At this critical point, the *critical compressibility factor*,  $Z_c$ , is:

$$Z_c = \frac{P_c V_c}{RT_c}$$

**TABLE 6.5** Critical Properties

| Substance            | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|----------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| Acetaldehyde         | 193        | 55          | 5.57        | 154                                         | 0.286                           |
| Acetic acid          | 319.56     | 57.1        | 5.786       | 171.3                                       | 0.351                           |
| Acetic anhydride     | 333        | 39.5        | 4.0         | 290                                         | 0.352                           |
| Acetone              | 235.0      | 46.4        | 4.700       | 209                                         | 0.278                           |
| Acetonitrile         | 272.4      | 47.7        | 4.85        | 173                                         | 0.237                           |
| Acetophenone         | 436.4      | 38          | 3.85        | 386                                         | 0.311                           |
| Acetyl chloride      | 235        | 58          | 5.88        | 204                                         | 0.325                           |
| Acetylene            | 35.2       | 60.6        | 6.14        | 113                                         | 0.231                           |
| Acrylic acid         | 342        | 56          | 5.67        | 210                                         | 0.343                           |
| Acrylonitrile        | 263        | 45          | 4.56        | 210                                         | 0.253                           |
| Air                  | -140.6     | 37.2        | 3.77        | 92.7                                        | 0.313                           |
| Allene               | 120        | 54.0        | 5.47        | 162                                         | 0.247                           |
| Allyl alcohol        | 272.0      | 56.4        | 5.71        | 203                                         | 0.286                           |
| Aluminum tribromide  | 490        | 28.5        | 2.89        | 310                                         | 0.860                           |
| Aluminum trichloride | 356        | 26          | 2.63        | 261                                         | 0.510                           |
| 2-Aminoethanol       | 341        | 44          | 4.46        | 196                                         | 0.312                           |
| Ammonia              | 132.4      | 111.3       | 11.28       | 72.5                                        | 0.235                           |
| Aniline              | 426        | 49.5        | 4.89        | 287                                         | 0.324                           |
| Anthracene           | 610        | 28.6        | 2.90        | 554                                         | 0.322                           |
| Antimony tribromide  | 631.4      | 56          | 5.67        |                                             |                                 |
| Antimony trichloride | 521        |             |             | 270                                         | 0.84                            |
| Argon                | -122.3     | 48.1        | 4.87        | 74.6                                        | 0.536                           |
| Arsenic              | 1400       |             |             |                                             |                                 |
| Arsenic trichloride  | 318        | 58.4        | 5.91        | 252                                         | 0.720                           |
| Arsine               | 99.9       | 63.3        | 6.41        | 133                                         | 0.588                           |
| Arsine- $d_3$        | 98.9       |             |             |                                             |                                 |
| Benzaldehyde         | 422        | 45.9        | 4.65        | 324                                         | 0.327                           |
| Benzene              | 288.90     | 48.31       | 4.895       | 255                                         | 0.306                           |
| Benzoic acid         | 479        | 41.55       | 4.21        | 341                                         | 0.358                           |
| Benzonitrile         | 426.3      | 41.55       | 4.21        | 339                                         | 0.304                           |
| Benzyl alcohol       | 422        | 42.4        | 4.3         | 334                                         | 0.324                           |
| Biphenyl             | 516        | 38.0        | 3.85        | 502                                         | 0.307                           |
| Bismuth tribromide   | 946        |             |             | 301                                         | 1.49                            |
| Bismuth trichloride  | 906        | 118         | 11.96       | 261                                         | 1.21                            |
| Boron pentafluoride  | 205        |             |             |                                             |                                 |
| Boron tribromide     | 308        | 48.1        | 4.87        | 272                                         | 0.921                           |
| Boron trichloride    | 178.8      | 38.2        | 3.87        | 266                                         | 0.441                           |



TABLE 6.5 Critical Properties (Continued)

| Substance                                 | $T_c, ^\circ\text{C}$ | $P_c, \text{atm}$ | $P_c, \text{MPa}$ | $V_c, \text{cm}^3 \cdot \text{mol}^{-1}$ | $\rho_c, \text{g} \cdot \text{cm}^{-3}$ |
|-------------------------------------------|-----------------------|-------------------|-------------------|------------------------------------------|-----------------------------------------|
| Boron trifluoride                         | − 12.3                | 49.2              | 4.98              | 124                                      | 0.549                                   |
| Bromine                                   | 315                   | 102               | 10.3              | 135                                      | 1.184                                   |
| Bromobenzene                              | 397                   | 44.6              | 4.52              | 324                                      | 0.485                                   |
| Bromochlorodifluoromethane                | 158.8                 | 41.98             | 4.254             | 246                                      | 0.672                                   |
| Bromoethane                               | 230.8                 | 61.5              | 6.23              | 215                                      | 0.507                                   |
| Bromomethane                              | 173.4                 | 85                | 8.61              | 156                                      | 0.609                                   |
| Bromopentafluorobenzene                   | 397                   | 44.6              | 4.52              |                                          |                                         |
| 1-Bromopropane                            | − 1.8                 |                   |                   |                                          | 0.462                                   |
| 2-Bromopropane                            | − 14.2                |                   |                   |                                          | 0.462                                   |
| Bromotrifluoromethane                     | 67.1                  | 39.2              | 3.97              | 200                                      | 0.76                                    |
| 1,2-Butadiene                             | 170.6                 | 44.4              | 4.50              | 219                                      | 0.247                                   |
| 1,3-Butadiene                             | 152                   | 42.7              | 4.33              | 221                                      | 0.245                                   |
| Butanal                                   | 264.1                 | 42.6              | 4.32              | 258                                      | 0.279                                   |
| Butane                                    | 151.97                | 37.34             | 3.784             | 255                                      | 0.228                                   |
| Butanenitrile                             | 312.3                 | 38.3              | 3.88              | 285                                      | 0.242                                   |
| Butanoic acid                             | 351                   | 39.8              | 4.03              | 290                                      | 0.304                                   |
| 1-Butanol                                 | 289.9                 | 43.56             | 4.414             | 275                                      | 0.270                                   |
| 2-Butanol                                 | 263.1                 | 41.47             | 4.202             | 269                                      | 0.276                                   |
| 2-Butanone                                | 263.63                | 41.52             | 4.207             | 267                                      | 0.270                                   |
| 1-Butene                                  | 146.5                 | 39.7              | 4.02              | 240                                      | 0.234                                   |
| cis-2-Butene                              | 147.5                 | 40.5              | 4.10              | 238                                      | 0.240                                   |
| trans-2-Butene                            | 147.5                 | 40.5              | 4.10              | 238                                      | 0.236                                   |
| 3-Butenenitrile                           | 312.3                 | 38.3              | 3.88              | 265                                      | 0.253                                   |
| 1-Buten-3-yne                             | 182                   | 49                | 4.96              | 202                                      | 0.258                                   |
| Butyl acetate                             | 306.7                 | 31                | 3.14              | 400                                      | 0.290                                   |
| 1-Butylamine                              | 258.8                 | 41.9              | 4.25              | 277                                      | 0.264                                   |
| sec-Butylamine                            | 241.2                 | 41.4              | 4.20              | 278                                      | 0.263                                   |
| tert-Butylamine                           | 210.8                 | 37.9              | 3.84              | 292                                      | 0.250                                   |
| Butylbenzene                              | 387.4                 | 28.5              | 2.89              | 497                                      | 0.270                                   |
| sec-Butylbenzene                          | 391                   | 29.1              | 2.94              | 510                                      | 0.263                                   |
| tert-Butylbenzene                         | 387                   | 29.3              | 2.97              | 490                                      | 0.273                                   |
| Butyl benzoate                            | 450                   | 26                | 2.63              | 561                                      | 0.318                                   |
| Butyl butanoate                           | 338                   |                   |                   |                                          | 0.292                                   |
| Butylcyclohexane                          | 394                   | 31.1              | 3.15              | 534                                      | 0.63                                    |
| sec-Butylcyclohexane                      | 396                   | 26.4              | 2.67              |                                          |                                         |
| tert-Butylcyclohexane                     | 385.9                 | 26.3              | 2.66              |                                          |                                         |
| Butylcyclopentane                         | 357.9                 |                   |                   |                                          |                                         |
| Butyl ethyl ether                         | 257.9                 | 30                | 3.04              | 390                                      | 0.262                                   |
| 2-Butylhexadecafluoro-<br>tetrahydrofuran | 227.1                 | 15.86             | 1.607             | 588                                      | 0.707                                   |
| Butylisopropylamine                       | 290.5                 |                   |                   |                                          |                                         |
| tert-Butyl methyl sulfide                 | 296.7                 |                   |                   |                                          |                                         |
| 1-Butyne                                  | 190.6                 | 46.5              | 4.71              | 220                                      | 0.246                                   |
| 2-Butyne                                  | 215.5                 | 50.2              | 5.09              | 221                                      | 0.246                                   |
| 4-Butyrolactone                           | 436                   |                   |                   |                                          |                                         |
| Carbon dioxide                            | 31.1                  | 72.8              | 7.38              | 94.0                                     | 0.468                                   |
| Carbon disulfide                          | 279                   | 78.0              | 7.90              | 173                                      | 0.41                                    |
| Carbon monoxide                           | − 140.2               | 34.5              | 3.50              | 93.1                                     | 0.301                                   |
| Carbon tetrachloride                      | 283.3                 | 45.0              | 4.56              | 276                                      | 0.558                                   |
| Carbon tetrafluoride                      | − 45.7                | 36.9              | 3.74              | 140                                      | 0.629                                   |
| Carbonyl chloride                         | 182                   | 56                | 5.67              | 190                                      | 0.52                                    |
| Carbonyl sulfide                          | 102                   | 58                | 5.88              | 140                                      | 0.44                                    |
| Cesium                                    | 1806                  |                   |                   | 300                                      | 0.44                                    |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                     | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|-------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| Chlorine                      | 143.8      | 76.1        | 7.71        | 124                                         | 0.573                           |
| Chlorine pentafluoride        | 142.6      | 51.9        | 5.26        | 230.9                                       | 0.565                           |
| Chlorine trifluoride          | 153.5      |             |             |                                             |                                 |
| Chlorobenzene                 | 359.3      | 44.6        | 4.52        | 308                                         | 0.365                           |
| 1-Chlorobutane                | 268.9      | 36.4        | 3.69        | 312                                         | 0.297                           |
| 2-Chlorobutane                | 247.5      | 39          | 3.95        | 305                                         | 0.303                           |
| 1-Chloro-1,1-difluoroethane   | 137.1      | 40.7        | 4.12        | 231                                         | 0.435                           |
| 2-Chloro-1,1-difluoroethylene | 127.5      | 44.0        | 4.46        | 197                                         | 0.499                           |
| Chlorodifluoromethane         | 96.1       | 49.1        | 4.98        | 165                                         | 0.525                           |
| 1-Chloro-2,3-epoxypropane     | 351        |             |             |                                             |                                 |
| Chloroethane                  | 187.3      | 52.0        | 5.27        | 199                                         | 0.324                           |
| Chloroform                    | 263.3      | 54.0        | 5.47        | 239                                         | 0.504                           |
| 1-Chlorohexane                | 321.5      |             |             |                                             |                                 |
| Chloromethane                 | 143.1      | 65.9        | 6.679       | 139                                         | 0.353                           |
| 2-Chloro-2-methylpropane      | 234        | 39          | 3.95        | 295                                         | 0.314                           |
| Chloropentafluoroacetone      | 137.6      | 28.4        | 2.88        |                                             |                                 |
| Chloropentafluorobenzene      | 297.9      | 31.8        | 3.22        |                                             |                                 |
| Chloropentafluoroethane       | 80.1       | 31.9        | 3.229       | 252                                         | 0.613                           |
| 1-Chloropentane               | 295.4      |             |             |                                             |                                 |
| 1-Chloropropane               | 230        | 45.2        | 4.58        | 254                                         | 0.309                           |
| 2-Chloropropane               | 212        | 46.6        | 4.72        | 230                                         | 0.341                           |
| 3-Chloropropene               | 241        | 47          | 4.76        | 234                                         | 0.336                           |
| Chlorotrifluoromethane        | 29         | 38.98       | 3.946       | 180                                         | 0.579                           |
| Chlorotrifluorosilane         | 35.4       |             | 3.47        |                                             |                                 |
| Chlorotrimethylsilane         | 224.7      | 31.6        | 3.20        |                                             |                                 |
| 1,2-Cresol                    | 424.5      | 49.4        | 5.01        | 282                                         | 0.384                           |
| 1,3-Cresol                    | 432.7      | 45.0        | 4.56        | 309                                         | 0.346                           |
| 1,4-Cresol                    | 431.5      | 50.8        | 5.15        | 277                                         | 0.391                           |
| Cyanogen                      | 126.7      | 62.2        | 6.30        | 145                                         | 0.360                           |
| Cyclobutane                   | 186.8      | 49.2        | 4.99        | 210                                         | 0.267                           |
| Cycloheptane                  | 316        | 36.7        | 3.72        | 390                                         | 0.252                           |
| Cyclohexane                   | 280.4      | 40.2        | 4.07        | 308                                         | 0.273                           |
| trans-Cyclohexanedimethanol   | 451        | 34.85       | 3.531       |                                             |                                 |
| Cyclohexanethiol              | 390.9      |             |             |                                             |                                 |
| Cyclohexanol                  | 376.9      | 42.0        | 4.26        | 327                                         | 0.306                           |
| Cyclohexanone                 | 379.9      | 39.5        | 4.0         | 312                                         | 0.315                           |
| Cyclohexene                   | 287.33     | 42.9        | 4.35        | 292                                         | 0.281                           |
| Cyclohexylamine               | 341.5      |             |             |                                             |                                 |
| Cyclopentane                  | 238.6      | 44.49       | 4.508       | 260                                         | 0.27                            |
| Cyclopentanethiol             | 360.4      |             |             |                                             |                                 |
| Cyclopentanone                | 353        | 53          | 5.37        | 268                                         | 0.314                           |
| Cyclopentene                  | 232.9      |             |             |                                             |                                 |
| 1-Cyclopentylheptane          | 406        | 19.2        | 1.94        | 649                                         | 0.260                           |
| 1-Cyclopentylpentadecane      | 506.9      | 10.1        | 1.02        | 1096                                        | 0.256                           |
| Cyclopropane                  | 124.7      | 54.2        | 5.49        | 170                                         | 0.248                           |
| p-Cymene                      | 379        | 2.80        | 2.84        | 492                                         | 0.273                           |
| Decafluorobutane              | 113.3      | 22.93       | 2.323       | 378                                         | 0.629                           |
| cis-Decahydronaphthalene      | 429.2      | 31.6        | 3.20        | 480                                         | 0.288                           |
| trans-Decahydronaphthalene    | 414.0      | 31          | 3.14        | 480                                         | 0.288                           |
| Decane                        | 344.6      | 20.8        | 2.11        | 624                                         | 0.228                           |
| Decanenitrile                 | 348.8      | 32.1        | 3.25        |                                             |                                 |
| 1-Decanol                     | 413.9      | 22          | 2.23        | 600                                         | 0.264                           |
| 1-Decene                      | 343.3      | 21.89       | 2.218       | 585                                         | 0.240                           |

TABLE 6.5 Critical Properties (Continued)

| Substance                            | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|--------------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| Decylcyclohexane                     | 477        | 13.4        | 1.36        |                                             |                                 |
| Decylcyclopentane                    | 450        | 15.0        | 1.52        |                                             |                                 |
| Deuterium (equilibrium)              | − 234.8    | 16.28       | 1.650       | 60.4                                        | 0.0668                          |
| Deuterium (normal)                   | − 234.7    | 16.43       | 1.665       | 60.3                                        | 0.0669                          |
| Deuterium bromide                    | 88.8       |             |             |                                             |                                 |
| Deuterium chloride                   | 50.3       |             |             |                                             |                                 |
| Deuterium hydride (DH)               | − 237.3    | 14.64       | 1.483       | 62.8                                        | 0.0481                          |
| Deuterium iodide                     | 148.6      |             |             |                                             |                                 |
| Deuterium oxide                      | 370.9      | 213.8       | 21.66       | 55.6                                        | 0.360                           |
| Diallyl sulfide                      | 380        |             |             |                                             |                                 |
| Diborane                             | 166        | 39.5        | 4.00        |                                             |                                 |
| 1,2-Dibromo-2-chlorotrifluoro-ethane | 287.6      |             |             |                                             |                                 |
| Dibromodifluoromethane               | 198.3      | 40.8        | 4.13        | 249                                         | 0.843                           |
| 1,2-Dibromoethane                    | 309.9      | 71.1        | 7.2         | 242                                         | 0.776                           |
| Dibromomethane                       | 310        | 71          | 7.19        |                                             |                                 |
| 1,2-Dibromotetrafluoroethane         | 214.7      | 33.49       | 3.393       | 329                                         | 0.790                           |
| Dibutylamine                         | 334.4      | 30.7        | 3.11        | 517                                         | 0.250                           |
| Dibutyl ether                        | 311.0      | 29.7        | 3.01        | 500                                         | 0.260                           |
| Dibutyl sulfide                      | 377        | 24.7        | 2.50        | 537                                         | 0.272                           |
| 1,2-Dichlorobenzene                  | 424.2      | 40.5        | 4.10        | 360                                         | 0.408                           |
| 1,3-Dichlorobenzene                  | 411        | 38          | 3.85        | 359                                         | 0.408                           |
| 1,4-Dichlorobenzene                  | 412        | 39          | 3.95        | 372                                         | 0.395                           |
| Dichlorodifluoromethane              | 111.80     | 40.82       | 4.136       | 217                                         | 0.558                           |
| 1,1-Dichloroethane                   | 250        | 50.0        | 5.07        | 236                                         | 0.419                           |
| Dichlorodifluorosilane               | 95.8       | 34.5        | 3.50        |                                             |                                 |
| 1,2-Dichloroethane                   | 288        | 53          | 5.4         | 225                                         | 0.440                           |
| 1,1-Dichloroethylene                 | 222        | 51.3        | 5.20        | 218                                         | 0.445                           |
| cis-1,2-Dichloroethylene             | 271.1      |             |             | 224                                         | 0.433                           |
| trans-1,2-Dichloroethylene           | 234.4      | 54.4        | 5.51        | 224                                         | 0.433                           |
| Dichlorofluoromethane                | 178.43     | 51.1        | 5.18        | 196                                         | 0.522                           |
| 1,2-Dichlorohexafluoropropane        | 172.9      |             |             |                                             |                                 |
| Dichloromethane                      | 237        | 60.2        | 6.10        | 193                                         | 0.440                           |
| 1,2-Dichloropropane                  | 304        | 44          | 4.49        | 226                                         | 0.500                           |
| Dichlorosilane                       | 176        | 46.1        | 4.67        |                                             |                                 |
| 1,1-Dichlorotetrafluoroethane        | 145.5      | 32.6        | 3.30        | 294                                         | 0.582                           |
| 1,2-Dichlorotetrafluoroethane        | 145.63     | 32.1        | 3.252       | 297                                         | 0.582                           |
| Dideuterium oxide (D <sub>2</sub> O) | 371.0      | 215.7       | 21.86       |                                             | 0.363                           |
| Diethanolamine                       | 442.0      | 32.3        | 3.27        | 349                                         | 0.301                           |
| 1,1-Diethoxyethane (Acetal)          | 254        |             |             |                                             |                                 |
| Diethylamine                         | 226.84     | 37.3        | 3.758       | 301                                         | 0.243                           |
| 1,4-Diethylbenzene                   | 384.8      | 27.7        | 2.81        | 480                                         | 0.280                           |
| Diethyl disulfide                    | 368.9      |             |             |                                             |                                 |
| Diethylene glycol                    | 408        | 46          | 4.66        | 316                                         | 0.336                           |
| Diethyl ether                        | 193.59     | 35.9        | 3.638       | 280                                         | 0.265                           |
| 3,3-Diethylhexane                    | 354.7      | 23.8        | 2.41        | 510                                         | 0.279                           |
| 3,4-Diethylhexane                    | 345.7      | 23.0        | 2.33        | 519                                         | 0.274                           |
| 3,3-Diethyl-2-methylpentane          | 366.8      | 25.0        | 2.53        | 501                                         | 0.284                           |
| 3,3-Diethylpentane                   | 337        | 26.4        | 2.67        |                                             |                                 |
| Diethyl sulfide                      | 284        | 39.1        | 3.96        | 318                                         | 0.284                           |
| Difluoroamine (HNF <sub>2</sub> )    | 130        | 93          | 9.42        |                                             |                                 |
| 1,2-Difluorobenzene                  | 284.2      |             |             | 300                                         | 0.381                           |
| cis-Difluorodiazine                  | − 1        | 70          | 7.09        |                                             |                                 |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                              | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|----------------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| <i>trans</i> -Difluorodiazine          | -13        | 55          | 5.57        |                                             |                                 |
| 1,1-Difluoroethane                     | 113.6      | 44.4        | 4.50        | 181                                         | 0.365                           |
| 1,1-Difluoroethylene                   | 29.8       | 44.0        | 4.46        | 154                                         | 0.417                           |
| Dihexyl ether                          | 384        | 18          | 1.82        | 720                                         | 0.259                           |
| Dihydrogen disulfide                   | 299        | 58.3        | 5.91        |                                             |                                 |
| Dihydrogen heptasulfide                | 742        | 33          | 3.34        |                                             |                                 |
| Dihydrogen hexasulfide                 | 707        | 36          | 3.65        |                                             |                                 |
| Dihydrogen octasulfide                 | 767        | 32          | 3.24        |                                             |                                 |
| Dihydrogen pentasulfide                | 657        | 38.4        | 3.89        |                                             |                                 |
| Dihydrogen tetrasulfide                | 582        | 43.1        | 4.37        |                                             |                                 |
| Dihydrogen trisulfide                  | 465        | 50.6        | 5.13        |                                             |                                 |
| Diisopentyl sulfide                    | 391        |             |             |                                             |                                 |
| Diisopropyl ether                      | 227.17     | 27.9        | 2.832       | 386                                         | 0.265                           |
| 1,2-Dimethoxyethane                    | 263        | 38.2        | 3.87        | 271                                         | 0.333                           |
| Dimethoxymethane                       | 242.1      | 44.2        | 4.48        |                                             |                                 |
| <i>N,N</i> -Dimethylacetamide          | 364        | 38.7        | 3.92        |                                             |                                 |
| Dimethylamine                          | 164.07     | 52.7        | 5.340       | 187                                         | 0.241                           |
| <i>N,N</i> -Dimethylaniline            | 414        | 35.8        | 3.63        |                                             |                                 |
| 2,2-Dimethylbutane                     | 215.7      | 30.49       | 3.090       | 359                                         | 0.240                           |
| 2,3-Dimethylbutane                     | 499.9      | 30.90       | 3.131       | 358                                         | 0.241                           |
| 3,3-Dimethyl-2-butanone                | 289.8      |             |             |                                             |                                 |
| 2,3-Dimethyl-1-butene                  | 228        | 32.0        | 3.24        | 343                                         | 0.245                           |
| 3,3-Dimethyl-1-butene                  | 217        | 32.1        | 3.25        | 340                                         | 0.248                           |
| 2,3-Dimethyl-2-butene                  | 250.9      | 33.2        | 3.36        | 351                                         | 0.240                           |
| 1,1-Dimethylcyclohexane                | 318        | 29.3        | 2.97        | 416                                         | 0.378                           |
| <i>cis</i> -1,2-Dimethylcyclohexane    | 333.0      | 29.0        | 2.94        | 460                                         | 0.244                           |
| <i>trans</i> -1,2-Dimethylcyclohexane  | 323.0      | 29.3        | 2.97        | 460                                         | 0.244                           |
| <i>cis</i> -1,3-Dimethylcyclohexane    | 317.9      | 29.3        | 2.97        | 450                                         | 0.249                           |
| <i>trans</i> -1,3-Dimethylcyclohexane  | 325        | 29.3        | 2.97        | 460                                         | 0.244                           |
| <i>cis</i> -1,4-Dimethylcyclohexane    | 325.0      | 29.0        | 2.94        | 460                                         | 0.244                           |
| <i>trans</i> -1,4-Dimethylcyclohexane  | 317.0      | 29.0        | 2.94        | 459                                         | 0.249                           |
| 1,1-Dimethylcyclopentane               | 274        | 34.0        | 3.44        | 360                                         | 0.273                           |
| <i>cis</i> -1,2-Dimethylcyclopentane   | 291.7      | 34.0        | 3.44        | 368                                         | 0.267                           |
| <i>trans</i> -1,2-Dimethylcyclopentane | 277.2      | 34.0        | 3.44        | 362                                         | 0.271                           |
| <i>cis</i> -1,3-Dimethylcyclopentane   | 318.9      |             |             |                                             |                                 |
| Dimethyl disulfide                     | 59.5       |             |             |                                             |                                 |
| Dimethyl ether                         | 126.9      | 53.0        | 5.37        | 190                                         | 0.242                           |
| <i>N,N</i> -Dimethylformamide          | 376.5      | 51.5        | 5.22        | 262                                         | 0.279                           |
| 2,2-Dimethylheptane                    | 303.7      | 23.19       | 2.350       | 519                                         | 0.247                           |
| 2,2-Dimethylhexane                     | 276.8      | 25.0        | 2.529       | 478                                         | 0.239                           |
| 2,3-Dimethylhexane                     | 290.4      | 25.94       | 2.628       | 468                                         | 0.244                           |
| 2,4-Dimethylhexane                     | 280.5      | 25.22       | 2.556       | 472                                         | 0.242                           |
| 2,5-Dimethylhexane                     | 277.0      | 24.54       | 2.487       | 482                                         | 0.237                           |
| 3,3-Dimethylhexane                     | 289.0      | 26.19       | 2.654       | 443                                         | 0.258                           |
| 3,4-Dimethylhexane                     | 295.8      | 26.57       | 2.692       | 466                                         | 0.245                           |
| 1,1-Dimethylhydrazine                  | 250        | 53.6        | 5.43        | 230                                         | 0.261                           |
| 2,4-Dimethyl-3-iso-pentane             | 341.3      | 23.1        | 2.34        | 521                                         | 0.273                           |
| 2,3-Dimethyloctane                     | 340.1      | 21.6        | 2.19        | 567                                         | 0.251                           |
| 2,4-Dimethyloctane                     | 326.3      | 21.1        | 2.14        | 566                                         | 0.251                           |
| 2,5-Dimethyloctane                     | 330        | 21.2        | 2.15        | 569                                         | 0.250                           |
| 2,6-Dimethyloctane                     | 330        | 21.1        | 2.15        | 576                                         | 0.247                           |
| 2,7-Dimethyloctane                     | 329.8      | 20.7        | 2.10        | 590                                         | 0.241                           |

TABLE 6.5 Critical Properties (Continued)

| Substance                  | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|----------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 3,3-Dimethyloctane         | 339        | 21.9        | 2.22        | 557                                         | 0.255                           |
| 3,4-Dimethyloctane         | 341        | 22.1        | 2.24        | 551                                         | 0.258                           |
| 3,5-Dimethyloctane         | 333.2      | 21.6        | 2.19        | 555                                         | 0.256                           |
| 3,6-Dimethyloctane         | 335.2      | 21.6        | 2.19        | 562                                         | 0.253                           |
| 4,5-Dimethyloctane         | 333.8      | 21.8        | 2.21        | 548                                         | 0.260                           |
| 4,5-Dimethyloctane         | 339.1      | 22.1        | 2.24        | 546                                         | 0.261                           |
| Dimethyl oxalate           | 355        | 39.2        | 3.97        |                                             |                                 |
| 2,2-Dimethylpentane        | 247.4      | 27.4        | 2.773       | 416                                         | 0.241                           |
| 2,3-Dimethylpentane        | 264.3      | 28.70       | 2.908       | 393                                         | 0.255                           |
| 2,4-Dimethylpentane        | 246.7      | 27.01       | 2.737       | 418                                         | 0.240                           |
| 3,3-Dimethylpentane        | 263.3      | 29.07       | 2.946       | 414                                         | 0.242                           |
| 2,3-Dimethylphenol         | 449.7      | 48          | 4.86        | 470                                         | 0.26                            |
| 2,4-Dimethylphenol         | 434.5      | 43          | 4.36        | 509                                         | 0.24                            |
| 2,5-Dimethylphenol         | 433.8      | 48          | 4.86        | 470                                         | 0.26                            |
| 2,6-Dimethylphenol         | 427.9      | 42          | 4.26        | 509                                         | 0.24                            |
| 3,4-Dimethylphenol         | 456.7      | 49          | 4.96        | 552                                         | 0.27                            |
| 3,5-Dimethylphenol         | 442.5      | 36          | 3.65        | 611                                         | 0.25                            |
| 2,2-Dimethylpropane        | 160.7      | 31.55       | 3.197       | 307                                         | 0.238                           |
| 2,2-Dimethyl-1-propanol    | 276        | 39          | 3.95        | 319                                         |                                 |
| 2,3-Dimethylpyridine       | 382.3      |             |             |                                             |                                 |
| 2,4-Dimethylpyridine       | 373.9      |             |             |                                             |                                 |
| 2,5-Dimethylpyridine       | 371        |             |             |                                             |                                 |
| 2,6-Dimethylpyridine       | 350.7      |             |             | 316                                         | 0.339                           |
| 3,4-Dimethylpyridine       | 410.7      |             |             |                                             |                                 |
| 3,5-Dimethylpyridine       | 394.1      |             |             |                                             |                                 |
| Dimethyl sulfide           | 229.9      | 54.6        | 5.53        | 201                                         | 0.309                           |
| N,N-Dimethyl-1,2-toluidine | 395        | 30.8        | 3.12        |                                             |                                 |
| 1,4-Dioxane                | 314        | 51.5        | 5.21        | 238                                         | 0.370                           |
| Diphenyl ether             | 493.7      | 31          | 3.14        |                                             |                                 |
| Diphenylmethane            | 494        | 29.4        | 2.98        |                                             |                                 |
| Dipropylamine              | 282.7      | 35.8        | 3.63        | 407                                         | 0.249                           |
| Dipropyl ether             | 257.5      | 29.91       | 3.028       |                                             |                                 |
| Docosafluorodecane         | 269        | 14.3        | 1.45        |                                             |                                 |
| Dodecafluorocyclohexane    | 184.1      | 24          | 2.43        |                                             |                                 |
| Dodecafluorocyclohexene    | 188.7      |             |             |                                             |                                 |
| Dodecafluoro-1-hexene      | 181.3      |             |             |                                             |                                 |
| Dodecafluoropentane        | 149        | 20.1        | 2.03        |                                             |                                 |
| Dodecane                   | 385        | 18.0        | 1.82        | 754                                         | 0.226                           |
| 1-Dodecanol                | 405.9      | 19          | 1.92        | 718                                         | 0.260                           |
| 1-Dodecene                 | 384.5      | 18.3        | 1.85        |                                             |                                 |
| Dodecylbenzene             | 501        | 15.6        | 1.58        | 1000                                        | 0.246                           |
| Dodecylcyclopentane        | 477        | 12.8        | 1.30        |                                             |                                 |
| Ethane                     | 32.3       | 48.2        | 4.90        | 148                                         | 0.203                           |
| 1,2-Ethanediamine          | 319.8      | 62.1        | 6.29        | 206                                         | 0.292                           |
| 1,2-Ethandiol              | 445        | 76          | 7.7         | 186                                         | 0.334                           |
| Ethanethiol                | 225.5      | 54.2        | 5.49        | 207                                         | 0.300                           |
| Ethanol                    | 240.9      | 60.57       | 6.137       | 167                                         | 0.276                           |
| Ethoxybenzene              | 374.0      | 33.8        | 3.42        |                                             |                                 |
| Ethyl acetate              | 250.2      | 38.31       | 3.882       | 286                                         | 0.308                           |
| Ethyl acetoacetate         | 400        |             |             |                                             |                                 |
| Ethyl acrylate             | 279        | 37.0        | 3.75        | 320                                         | 0.313                           |
| Ethylamine                 | 183        | 55.5        | 5.62        | 182                                         | 0.248                           |
| Ethylbenzene               | 344.00     | 35.61       | 3.609       | 374                                         | 0.284                           |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                              | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|----------------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| Ethyl benzoate                         | 424        | 32          | 3.24        | 451                                         | 0.111                           |
| Ethylbutanoate                         | 293        | 30.2        | 3.06        | 421                                         | 0.28                            |
| 2-Ethyl-1-butanol                      | 145.7      |             |             |                                             |                                 |
| Ethyl crotonate                        | 326        |             |             |                                             |                                 |
| Ethylcyclohexane                       | 336        | 29.9        | 3.03        | 450                                         | 0.249                           |
| Ethylcyclopentane                      | 296.4      | 33.5        | 3.39        | 375                                         | 0.262                           |
| 3-Ethyl-2,2-dimethylhexane             | 338.6      | 22.8        | 2.31        | 526                                         | 0.271                           |
| 4-Ethyl-2,2-dimethylhexane             | 321.5      | 21.9        | 2.22        | 539                                         | 0.264                           |
| 3-Ethyl-2,3-dimethylhexane             | 353.7      | 23.9        | 2.42        | 516                                         | 0.276                           |
| 4-Ethyl-2,3-dimethylhexane             | 344.2      | 23.1        | 2.34        | 524                                         | 0.271                           |
| 3-Ethyl-2,4-dimethylhexane             | 343.0      | 23.1        | 2.34        | 522                                         | 0.273                           |
| 4-Ethyl-2,4-dimethylhexane             | 347.8      | 24.4        | 2.47        | 524                                         | 0.271                           |
| 3-Ethyl-2,5-dimethylhexane             | 330.4      | 22.1        | 2.24        | 537                                         | 0.265                           |
| 3-Ethyl-3,4-dimethylhexane             | 351.4      | 23.9        | 2.42        | 511                                         | 0.278                           |
| Ethylene                               | 9.3        | 49.7        | 5.036       | 129                                         | 0.218                           |
| Ethylene glycol dimethyl ether         | 263        | 38.2        | 3.87        | 271                                         | 0.333                           |
| Ethylene glycol ethyl ether<br>acetate | 334.2      | 31.25       | 3.166       | 443                                         | 0.298                           |
| Ethylene glycol monobutyl<br>ether     | 360.8      |             |             | 424                                         | 0.279                           |
| Ethylene oxide                         | 196        | 71.0        | 7.275       | 140                                         | 0.314                           |
| Ethyl formate                          | 235.4      | 46.8        | 4.74        | 229                                         | 0.323                           |
| 3-Ethylhexane                          | 292.4      | 25.74       | 2.608       | 455                                         | 0.251                           |
| 2-Ethyl-1-hexanol                      | 367.5      | 27.2        | 2.76        | 494                                         | 0.264                           |
| Ethyl isopentanoate                    | 315        |             |             |                                             |                                 |
| Ethyl isopropyl ether                  | 217.2      |             |             |                                             |                                 |
| 2-Ethyl-1-methylbenzene                | 378        | 30.0        | 3.04        | 460                                         | 0.26                            |
| 3-Ethyl-1-methylbenzene                | 364        | 28.0        | 2.84        | 490                                         | 0.24                            |
| 4-Ethyl-1-methylbenzene                | 367        | 29.0        | 2.94        | 470                                         | 0.26                            |
| Ethyl 3-methylbutanoate                | 314.9      |             |             |                                             |                                 |
| 1-Ethyl-1-methylcyclopentane           | 319        | 29.5        | 2.99        |                                             |                                 |
| Ethyl methyl ether                     | 164.8      | 43.4        | 4.40        | 221                                         | 0.272                           |
| 3-Ethyl-2-methylheptane                | 337.8      | 22.0        | 2.23        | 544                                         | 0.262                           |
| 4-Ethyl-2-methylheptane                | 328.7      | 21.6        | 2.19        | 545                                         | 0.261                           |
| 5-Ethyl-2-methylheptane                | 333.6      | 21.6        | 2.19        | 555                                         | 0.256                           |
| 3-Ethyl-3-methylheptane                | 347.0      | 22.8        | 2.31        | 532                                         | 0.267                           |
| 4-Ethyl-3-methylheptane                | 341.2      | 22.5        | 2.28        | 530                                         | 0.269                           |
| 5-Ethyl-3-methylheptane                | 333.5      | 22.0        | 2.23        | 541                                         | 0.263                           |
| 3-Ethyl-4-methylheptane                | 342.4      | 22.5        | 2.28        | 533                                         | 0.267                           |
| 4-Ethyl-4-methylheptane                | 342.4      | 22.8        | 2.31        | 525                                         | 0.271                           |
| Ethyl methyl ketone                    | 262.4      | 41.0        | 4.154       | 267                                         | 0.270                           |
| 3-Ethyl-2-methylpentane                | 294.0      | 26.65       | 2.700       | 443                                         | 0.258                           |
| 3-Ethyl-3-methylpentane                | 303.5      | 27.71       | 2.808       | 455                                         | 0.351                           |
| Ethyl 2-methylpropanoate               | 280        | 30          | 3.04        | 410                                         | 0.28                            |
| Ethyl methyl sulfide                   | 260        | 42          | 4.26        |                                             |                                 |
| 2-Ethyl-naphthalene                    | 502        | 31.0        | 3.14        | 521                                         | 0.300                           |
| Ethyl nonanoate                        | 401        |             |             |                                             |                                 |
| 3-Ethyl-octane                         | 340        | 21.6        | 2.19        | 561                                         | 0.241                           |
| 4-Ethyl-octane                         | 337        | 21.5        | 2.18        | 552                                         | 0.258                           |
| Ethyl octanoate                        | 386        |             |             |                                             |                                 |
| 3-Ethyl-pentane                        | 267.6      | 28.53       | 2.891       | 416                                         | 0.241                           |
| 1,2-Ethylphenol                        | 429.9      |             |             |                                             |                                 |
| 1,3-Ethylphenol                        | 443.3      |             |             |                                             |                                 |

TABLE 6.5 Critical Properties (Continued)

| Substance                           | $T_c, ^\circ\text{C}$ | $P_c, \text{atm}$ | $P_c, \text{MPa}$ | $V_c, \text{cm}^3 \cdot \text{mol}^{-1}$ | $\rho_c, \text{g} \cdot \text{cm}^{-3}$ |
|-------------------------------------|-----------------------|-------------------|-------------------|------------------------------------------|-----------------------------------------|
| 1,4-Ethylphenol                     | 443.3                 |                   |                   |                                          |                                         |
| Ethyl propanoate                    | 272.9                 | 33.18             | 3.362             | 345                                      | 0.296                                   |
| Ethyl propyl ether                  | 227.1                 | 32.1              | 3.25              | 244                                      | 0.361                                   |
| <i>m</i> -Ethyltoluene              | 364.0                 | 28.1              | 2.837             | 490                                      | 0.245                                   |
| <i>o</i> -Ethyltoluene              | 378.0                 | 30.1              | 3.04              | 460                                      | 0.261                                   |
| <i>p</i> -Ethyltoluene              | 367                   | 29.0              | 2.94              | 479                                      | 0.256                                   |
| 3-Ethyl-2,2,3-trimethyl-<br>pentane | 372.9                 | 25.4              | 2.57              | 503                                      | 0.283                                   |
| 3-Ethyl-2,2,4-trimethyl-<br>pentane | 342.2                 | 23.4              | 2.37              | 518                                      | 0.275                                   |
| 3-Ethyl-2,3,4-trimethyl-<br>pentane | 369.2                 | 25.1              | 2.54              | 506                                      | 0.281                                   |
| Ethyl vinyl ether                   | 202                   | 40.17             | 4.07              | 260                                      | 0.277                                   |
| Fluorine                            | −129.0                | 51.47             | 5.215             | 66.2                                     | 0.574                                   |
| Fluorobenzene                       | 286.94                | 44.91             | 4.551             | 357                                      | 0.269                                   |
| Fluoroethane                        | 102.2                 | 49.6              | 5.03              | 169                                      | 0.284                                   |
| Fluoromethane                       | 44.7                  | 58.0              | 5.88              | 124                                      | 0.274                                   |
| 4-Fluorotoluene                     | 316.4                 |                   |                   |                                          |                                         |
| Formaldehyde                        | 135                   | 65                | 6.6               | 105                                      | 0.286                                   |
| Formic acid                         | 315                   |                   |                   |                                          |                                         |
| 2-Furaldehyde                       | 397                   | 58.1              | 5.89              |                                          |                                         |
| Furan                               | 217.1                 | 54.3              | 5.50              | 218                                      | 0.312                                   |
| Germanium tetrachloride             | 276.9                 | 38                | 3.85              | 330                                      | 0.650                                   |
| Glycerol                            | 453                   | 66                | 6.69              | 255                                      | 0.361                                   |
| Hafnium tetrabromide                | 473                   |                   |                   | 415                                      | 1.20                                    |
| Hafnium tetrachloride               | 450                   | 57.0              | 5.86              | 304                                      | 1.05                                    |
| Hafnium tetraiodide                 | 643                   |                   |                   | 528                                      | 1.30                                    |
| Helium (equilibrium)                | −267.96               | 2.261             | 0.2289            |                                          | 0.06930                                 |
| Helium-3                            | −269.85               | 1.13              | 0.1182            | 72.5                                     | 0.0414                                  |
| Helium-4                            | −267.96               | 2.24              | 0.227             | 57.3                                     | 0.0698                                  |
| Heptadecane                         | 460                   | 13.0              | 1.32              | 1006                                     | 0.140                                   |
| 1-Heptadecanol                      | 736                   | 14.0              | 1.42              | 960                                      | 0.267                                   |
| Heptane                             | 267.1                 | 27.0              | 2.74              | 428                                      | 0.232                                   |
| 1-Heptanol                          | 359.5                 | 30.18             | 3.058             | 435                                      | 0.267                                   |
| 2-Heptanol                          | 335.2                 | 29.81             | 3.021             | 432                                      | 0.269                                   |
| 3-Heptanol                          | 332.3                 |                   |                   |                                          |                                         |
| 2-Heptanone                         | 338.4                 | 33.91             | 3.436             | 421                                      | 0.271                                   |
| 1-Heptene                           | 264.2                 | 28.83             | 2.921             | 402                                      | 0.246                                   |
| Heptylcyclopentane                  | 406                   | 19.2              | 1.945             |                                          |                                         |
| Hexadecafluoroheptane               | 201.7                 | 16.0              | 1.62              | 664                                      | 0.584                                   |
| Hexadecane                          | 444                   | 14                | 1.42              | 930                                      | 0.243                                   |
| 1-Hexadecene                        | 444                   | 13.2              | 1.34              | 933                                      | 0.241                                   |
| Hexadecylcyclopentane               | 518                   | 9.6               | 0.97              |                                          |                                         |
| 1,5-Hexadiene                       | 234                   | 34                | 3.44              | 328                                      | 0.250                                   |
| Hexafluoroacetone                   | 84.1                  | 29.0              | 2.94              | 329                                      | 0.505                                   |
| Hexafluorobenzene                   | 243.6                 | 32.30             | 3.273             | 335                                      | 0.505                                   |
| Hexafluoroethane                    | 19.7                  |                   |                   | 224                                      | 0.617                                   |
| Hexamethylbenzene                   | 494                   |                   |                   | 600                                      | 0.271                                   |
| Hexane                              | 234.5                 | 29.85             | 3.025             | 368                                      | 0.233                                   |
| Hexanenitrile                       | 360.7                 | 32.57             | 3.30              |                                          |                                         |
| Hexanoic acid                       | 389                   | 31.6              | 3.20              |                                          |                                         |
| 1-Hexanol                           | 337.2                 | 33.72             | 3.417             | 381                                      | 0.268                                   |
| 2-Hexanol                           | 312.8                 | 32.67             | 3.310             |                                          |                                         |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                   | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|-----------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 3-Hexanol                   | 309.3      | 33.2        | 3.36        |                                             |                                 |
| 2-Hexanone                  | 313.9      | 32.8        | 3.32        |                                             |                                 |
| 3-Hexanone                  | 309.7      | 32.76       | 3.320       |                                             |                                 |
| 1-Hexene                    | 231.0      | 31.64       | 3.206       | 348                                         | 0.242                           |
| <i>cis</i> -2-Hexene        | 245        | 32.4        | 3.28        | 351                                         | 0.240                           |
| <i>trans</i> -2-Hexene      | 243        | 32.3        | 3.27        | 351                                         | 0.240                           |
| <i>cis</i> -3-Hexene        | 244        | 32.4        | 3.28        | 350                                         | 0.240                           |
| <i>trans</i> -3-Hexene      | 246.8      | 32.1        | 3.25        | 350                                         | 0.240                           |
| Hexylcyclopentane           | 387.0      | 21.1        | 2.14        |                                             |                                 |
| Hydrazine                   | 380        | 14.5        | 1.47        | 96.1                                        | 0.333                           |
| Hydrogen (equilibrium)      | -240.17    | 12.77       | 1.294       | 65.4                                        | 0.0308                          |
| Hydrogen (normal)           | -239.91    | 12.8        | 1.297       | 65.0                                        | 0.0310                          |
| Hydrogen bromide            | 89.8       | 84.4        | 8.55        | 100.0                                       | 0.809                           |
| Hydrogen chloride           | 51.40      | 82.0        | 8.31        | 81.0                                        | 0.45                            |
| Hydrogen cyanide            | 183.5      | 53.2        | 5.39        | 139                                         | 0.195                           |
| Hydrogen deuteride          | -237.25    | 14.64       | 1.483       | 62.8                                        | 0.048                           |
| Hydrogen fluoride           | 188        | 64          | 6.5         | 69                                          | 0.29                            |
| Hydrogen iodide             | 150.7      | 82.0        | 8.31        | 131                                         | 0.976                           |
| Hydrogen selenide           | 137        | 88          | 8.9         |                                             |                                 |
| Hydrogen sulfide            | 100.4      | 88.2        | 8.94        | 98.5                                        | 0.31                            |
| Icosafluorononane           | 251        | 15.4        | 1.56        |                                             |                                 |
| Icosane                     | 494        | 10.3        | 1.04        | 1190                                        | 0.237                           |
| 1-Icosanol                  | 497        | 12.0        | 1.22        |                                             |                                 |
| Indane                      | 411.8      | 39.0        | 3.95        | 381                                         | 0.310                           |
| Iodine                      | 546        | 115         | 11.7        | 155                                         | 0.164                           |
| Iodobenzene                 | 448        | 44.6        | 4.52        | 351                                         | 0.581                           |
| Iodoethane                  | 281.0      |             |             |                                             |                                 |
| Iodomethane                 | 255        | 65          | 6.59        | 190                                         | 0.75                            |
| 1-Iodopropane               | 323        |             |             |                                             |                                 |
| Isobutyl acetate            | 288        | 31.2        | 3.16        | 414                                         | 0.281                           |
| Isobutylamine               | 246        | 40.2        | 4.07        | 284                                         | 0.258                           |
| Isobutylbenzene             | 377        | 30.1        | 3.05        | 480                                         | 0.280                           |
| Isobutyl bromide            | 294.1      |             |             |                                             |                                 |
| Isobutyl butanoate          | 338        |             |             |                                             |                                 |
| Isobutylcyclohexane         | 386        | 30.8        | 3.12        |                                             |                                 |
| Isobutyl formate            | 278        | 38.3        | 3.88        | 350                                         | 0.29                            |
| Isobutyl isobutanoate       | 329        |             |             |                                             |                                 |
| Isobutyl 3-methylbutanoate  | 348        |             |             |                                             |                                 |
| Isobutyl propanoate         | 319        |             |             |                                             |                                 |
| Isopentyl acetate           | 326        |             |             |                                             |                                 |
| Isopentyl butanoate         | 346        |             |             |                                             |                                 |
| Isopentyl propanoate        | 338        |             |             |                                             |                                 |
| Isopropyl acetate           | 258        |             |             |                                             |                                 |
| Isopropylamine              | 198.7      | 44.8        | 4.54        | 221                                         | 0.267                           |
| Isopropylbenzene            | 357.9      | 31.67       | 3.209       | 429                                         | 0.281                           |
| Isopropylcycloheptane       | 334.5      |             |             |                                             |                                 |
| Isopropylcyclohexane        | 367        | 28          | 2.84        |                                             |                                 |
| Isopropylcyclopentane       | 328        | 29.6        | 3.00        |                                             |                                 |
| 4-Isopropylheptane          | 334.5      | 22.0        | 2.23        | 537                                         | 0.265                           |
| Isopropylmethylamine        | 217.6      |             |             |                                             |                                 |
| 2-Isopropyl-1-methylbenzene | 397        | 28.6        | 2.90        |                                             |                                 |
| 3-Isopropyl-1-methylbenzene | 393        | 29.0        | 2.94        |                                             |                                 |
| 4-Isopropyl-1-methylbenzene | 380        | 27.9        | 2.83        |                                             |                                 |



TABLE 6.5 Critical Properties (Continued)

| Substance                  | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|----------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 3-Isopropyl-2-methylhexane | 359.3      | 22.6        | 2.29        | 529                                         | 0.269                           |
| Isopropyl methyl sulfide   | 276.4      |             |             |                                             |                                 |
| Isoquinoline               | 530        | 50.3        | 5.10        | 374                                         | 0.345                           |
| Isoxazole                  | 278.9      |             |             |                                             |                                 |
| Ketene                     | 380        | 64          | 6.5         | 145                                         | 0.290                           |
| Krypton                    | - 63.75    | 54.3        | 5.50        | 91.2                                        | 0.9085                          |
| Mercury                    | 1477       | 1587        | 160.8       |                                             |                                 |
| Mercury(II) bromide        | 789        |             |             |                                             |                                 |
| Mercury(II) chloride       | 700        |             |             |                                             |                                 |
| Mercury(II) iodide         | 799        |             |             |                                             |                                 |
| Methane                    | - 82.60    | 45.44       | 4.604       | 99.0                                        | 0.162                           |
| Methanethiol               | 196.8      | 71.4        | 7.23        | 145                                         | 0.332                           |
| Methanol                   | 239.4      | 79.78       | 8.084       | 118                                         | 0.272                           |
| Methoxybenzene             | 372.5      | 41.9        | 4.25        |                                             | 0.321                           |
| Methyl acetamide           | 417        |             |             |                                             |                                 |
| Methyl acetate             | 233.40     | 46.9        | 4.75        | 228                                         | 0.325                           |
| Methyl acrylate            | 263        | 42          | 4.26        | 265                                         | 0.325                           |
| Methylamine                | 157.6      | 75.14       | 7.614       | 140                                         | 0.222                           |
| N-Methylaniline            | 428        | 51.3        | 5.20        | 373                                         | 0.287                           |
| Methyl benzoate            | 438        | 36          | 3.65        | 396                                         | 0.344                           |
| 2-Methyl-1,3-butadiene     | 211        | 38.0        | 3.85        | 276                                         | 0.247                           |
| 3-Methyl-1,3-butadiene     | 223        | 40.6        | 4.11        | 267                                         | 0.255                           |
| 2-Methylbutane             | 187.3      | 33.4        | 3.38        | 306                                         | 0.236                           |
| 2-Methyl-1-butanethiol     | 318.8      |             |             |                                             |                                 |
| 2-Methyl-2-butanethiol     | 297.0      |             |             |                                             |                                 |
| Methyl butanoate           | 281.3      | 34.3        | 3.475       | 340                                         | 0.300                           |
| 3-Methylbutanoic acid      | 356        | 33.6        | 3.40        |                                             |                                 |
| 2-Methyl-1-butanol         | 302.3      | 38.9        | 3.94        | 322                                         | 0.274                           |
| 3-Methyl-1-butanol         | 304.1      | 38.8        | 3.93        | 329                                         | 0.268                           |
| 2-Methyl-2-butanol         | 270.6      | 36.6        | 3.71        | 319                                         | 0.276                           |
| 3-Methyl-2-butanol         | 283.0      | 38.2        | 3.87        |                                             |                                 |
| 3-Methyl-2-butanone        | 280.3      | 38.0        | 3.85        | 310                                         | 0.278                           |
| 2-Methyl-1-butene          | 196.9      | 34.0        | 3.445       | 294                                         | 0.239                           |
| 3-Methyl-1-butene          | 191.6      | 34.7        | 3.52        | 300                                         | 0.234                           |
| 2-Methyl-2-butene          | 207.9      | 34.0        | 3.445       | 318                                         | 0.221                           |
| Methylcyclohexane          | 299.1      | 34.26       | 3.471       | 368                                         | 0.267                           |
| Methylcyclopentane         | 259.58     | 37.35       | 3.784       | 319                                         | 0.264                           |
| Methyl dodecanoate         | 439        |             |             | 758                                         | 0.283                           |
| N-Methylethylamine         | 223.5      | 36.6        | 3.71        | 243                                         | 0.243                           |
| Methyl formate             | 214.1      | 59.20       | 5.998       | 172                                         | 0.349                           |
| 2-Methylfuran              | 254        | 46.6        | 4.72        | 247                                         | 0.333                           |
| 2-Methylheptane            | 286.6      | 24.52       | 2.484       | 488                                         | 0.234                           |
| 3-Methylheptane            | 290.6      | 25.13       | 2.546       | 464                                         | 0.246                           |
| 4-Methylheptane            | 288.7      | 25.09       | 2.542       | 476                                         | 0.240                           |
| 2-Methylhexane             | 257.3      | 26.98       | 2.734       | 421                                         | 0.238                           |
| 3-Methylhexane             | 262.2      | 27.77       | 2.814       | 404                                         | 0.248                           |
| Methylhydrazine            | 294        | 79.3        | 8.035       | 271                                         | 0.170                           |
| Methyl 2-hydroxybenzoate   | 436        |             |             |                                             |                                 |
| Methyl isobutanoate        | 267.7      | 33.9        | 3.43        | 339                                         | 0.301                           |
| Methyl isocyanate          | 218        | 55          | 5.57        |                                             |                                 |
| 1-Methylnaphthalene        | 499        | 35.5        | 3.60        | 445                                         | 0.320                           |
| 2-Methylnaphthalene        | 488        | 34.6        | 3.51        | 462                                         | 0.308                           |
| 2-Methyloctane             | 313.9      | 22.80       | 2.310       |                                             |                                 |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                                | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|------------------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 2-Methylpentane                          | 224.6      | 29.91       | 3.031       | 367                                         | 0.235                           |
| 3-Methylpentane                          | 231.4      | 30.85       | 3.126       | 367                                         | 0.235                           |
| 2-Methyl-2,4-pentanediol                 | 405        | 33.9        | 3.43        |                                             |                                 |
| Methyl pentanoate                        | 294        |             |             |                                             |                                 |
| 2-Methyl-2-pentanol                      | 286.4      |             |             |                                             |                                 |
| 2-Methyl-3-pentanol                      | 302.9      | 34.1        | 3.46        |                                             |                                 |
| 3-Methyl-3-pentanol                      | 302.5      | 34.7        | 3.52        |                                             |                                 |
| 4-Methyl-1-pentanol                      | 330.4      |             |             |                                             |                                 |
| 4-Methyl-2-pentanol                      | 301.3      | 42.4        | 4.30        | 380                                         | 0.269                           |
| 3-Methyl-2-pentanone                     | 298.8      |             |             |                                             |                                 |
| 4-Methyl-2-pentanone                     | 298        | 32.3        | 3.27        | 371                                         | 0.270                           |
| 2-Methyl-2-pentene                       | 245        | 32.4        | 3.28        | 351                                         | 0.240                           |
| <i>cis</i> -3-Methyl-2-pentene           | 245        | 32.4        | 3.28        | 351                                         | 0.240                           |
| <i>trans</i> -3-Methyl-2-pentene         | 248        | 32.3        | 3.27        | 350                                         | 0.240                           |
| <i>cis</i> -4-Methyl-2-pentene           | 217        | 30          | 3.04        | 360                                         | 0.234                           |
| <i>trans</i> -4-Methyl-2-pentene         | 220        | 30          | 3.04        | 360                                         | 0.234                           |
| 2-Methylpropanal                         | 240        | 41          | 4.15        | 274                                         | 0.263                           |
| 2-Methyl-1-propanamine                   | 246        | 40.2        | 4.07        | 278                                         | 0.263                           |
| <i>N</i> -Methylpropanamide              | 412        |             |             |                                             |                                 |
| 2-Methylpropane                          | 134.70     | 35.83       | 3.630       | 263                                         | 0.221                           |
| 2-Methyl-1-propanethiol                  | 286.4      |             |             |                                             |                                 |
| 2-Methyl-2-propanethiol                  | 257.0      |             |             |                                             |                                 |
| Methyl propanoate                        | 257.5      | 39.5        | 4.00        | 282                                         | 0.312                           |
| 2-Methylpropanoic acid                   | 332        | 36.5        | 3.7         | 292                                         | 0.302                           |
| 2-Methyl-1-propanol                      | 274.6      | 42.39       | 4.295       | 273                                         | 0.272                           |
| 2-Methyl-2-propanol                      | 233.1      | 39.20       | 3.972       | 275                                         | 0.270                           |
| 2-Methylpropene                          | 144.73     | 39.48       | 4.000       | 239                                         | 0.235                           |
| 2-Methylpropyl acetate                   | 288        | 31.2        | 3.16        | 414                                         | 0.281                           |
| Methyl propyl ether                      | 203.2      |             |             |                                             |                                 |
| Methyl propyl sulfide                    | 301.0      |             |             |                                             |                                 |
| 2-Methylpyridine                         | 347.9      | 45.4        | 4.60        | 292                                         | 0.319                           |
| 3-Methylpyridine                         | 371.9      | 44.2        | 4.48        | 288                                         | 0.323                           |
| 4-Methylpyridine                         | 373        | 46.4        | 4.70        | 292                                         | 0.319                           |
| 1-Methyl-2-pyrrolidinone                 | 448.7      |             |             | 311                                         | 0.319                           |
| 1-Methylstyrene                          | 381        | 33.6        | 3.40        | 397                                         | 0.298                           |
| 2-Methyltetrahydrofuran                  | 264        | 37.1        | 3.76        | 267                                         | 0.322                           |
| 2-Methylthiophene                        | 333.1      | 47.9        | 4.85        | 275                                         | 0.356                           |
| 3-Methylthiophene                        | 337.7      | 48.9        | 4.95        | 275                                         | 0.356                           |
| Methyl vinyl ether                       | 163        | 47          | 4.76        | 205                                         | 0.283                           |
| Morpholine                               | 345        | 54          | 54.7        | 253                                         | 0.344                           |
| Naphthalene                              | 475.3      | 39.98       | 4.051       | 407                                         | 0.31                            |
| Neon                                     | -228.71    | 27.2        | 2.77        | 41.7                                        | 0.4835                          |
| Niobium pentabromide                     | 737        |             |             | 469                                         | 1.05                            |
| Niobium pentachloride                    | 534        |             |             | 400                                         | 0.68                            |
| Niobium pentafluoride                    | 464        | 62          | 6.28        | 155                                         | 1.21                            |
| Nitric oxide                             | -92.9      | 64.6        | 6.55        | 58                                          | 0.52                            |
| Nitrobenzene                             | 459        |             |             |                                             |                                 |
| Nitroethane                              | 284        | 37          | 3.75        |                                             |                                 |
| Nitrogen-14                              | 146.94     | 33.5        | 3.39        | 89.5                                        | 0.313                           |
| Nitrogen-15                              | 146.8      | 33.5        | 3.39        | 90.4                                        | 0.332                           |
| Nitrogen chloride difluoride             | 64.3       | 50.8        | 5.15        |                                             |                                 |
| Nitrogen dioxide (equilibrium)           | 158.2      | 100         | 10.1        | 170                                         | 0.557                           |
| Nitrogen trideuteride (ND <sub>3</sub> ) | 132.4      |             |             |                                             |                                 |

TABLE 6.5 Critical Properties (Continued)

| Substance                         | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|-----------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| Nitrogen trifluoride              | − 39.3     | 44.7        | 4.53        |                                             |                                 |
| Nitromethane                      | 315        | 57.9        | 5.87        | 173                                         | 0.352                           |
| 1-Nitropropane                    | 402.0      |             |             |                                             |                                 |
| 2-Nitropropane                    | 344.8      |             |             |                                             |                                 |
| Nitrous oxide                     | 36.434     | 71.596      | 7.2545      | 97.4                                        | 0.4525                          |
| Nitrosyl chloride                 | 167        | 90          | 9.12        | 139                                         | 0.471                           |
| Nitryl fluoride                   | 76.3       |             |             |                                             |                                 |
| Nonadecane                        | 483        | 11.0        | 1.12        | 1130                                        | 0.238                           |
| Nonane                            | 321.5      | 22.6        | 2.29        | 555                                         | 0.231                           |
| Nonanoic acid                     | 438        | 23.7        | 2.40        |                                             |                                 |
| 1-Nonanol                         | 404        |             |             | 546                                         | 0.264                           |
| 1-Nonene                          | 319        | 23.1        | 2.34        | 580                                         | 0.218                           |
| Nonylbenzene                      | 468        | 18.7        | 1.89        | 790                                         | 0.259                           |
| Nonylcyclopentane                 | 437.4      | 16.3        | 1.65        |                                             |                                 |
| Octadecafluorooctane              | 229        | 16.4        | 1.66        |                                             |                                 |
| Octadecane                        | 472.3      | 12.73       | 1.29        | 1070                                        | 0.238                           |
| 1-Octadecanol                     | 474        | 14          | 1.42        |                                             |                                 |
| 1-Octadecene                      | 466        | 11.2        | 1.13        |                                             |                                 |
| Octafluorocyclobutane             | 115.31     | 27.48       | 2.784       | 325                                         | 0.616                           |
| Octafluoronaphthalene             | 399.9      |             |             |                                             |                                 |
| Octafluoropropane                 | 72.7       | 26.5        | 2.69        | 299                                         | 0.628                           |
| Octamethylcyclotetrasiloxane      | 313        | 13.2        | 1.33        | 970                                         | 0.306                           |
| Octane                            | 295.6      | 24.6        | 2.49        | 492                                         | 0.232                           |
| Octanenitrile                     | 401.3      | 28.1        | 2.85        |                                             |                                 |
| Octanoic acid                     | 422        | 26.1        | 2.64        |                                             |                                 |
| 1-Octanol                         | 379.4      | 27.41       | 2.777       | 490                                         | 0.266                           |
| 2-Octanol                         | 356.5      | 27.18       | 2.754       | 494                                         | 0.278                           |
| 1-Octene                          | 293.6      | 26.40       | 2.675       | 464                                         | 0.242                           |
| cis-2-Octene                      | 307        | 27.3        | 2.77        |                                             |                                 |
| Octylcyclopentane                 | 421        | 17.7        | 1.79        |                                             |                                 |
| Osmium tetroxide                  | 132        | 170         | 17.2        |                                             |                                 |
| Oxygen                            | − 118.56   | 49.77       | 5.043       | 73.4                                        | 0.436                           |
| Oxygen difluoride                 | − 58.0     | 48.9        | 4.95        | 97.7                                        | 0.553                           |
| Ozone                             | − 12.10    | 53.8        | 5.45        | 88.9                                        | 0.540                           |
| Pentachloroethane                 | 373.0      |             |             |                                             |                                 |
| Pentadecane                       | 433.9      | 15          | 1.52        | 880                                         | 0.241                           |
| 1-Pentadecene                     | 431        | 14.4        | 1.46        |                                             |                                 |
| Pentadecylcyclopentane            | 507        | 10.1        | 1.02        |                                             |                                 |
| 1,2-Pentadiene                    | 230        | 40.2        | 4.07        | 276                                         | 0.248                           |
| cis-1,3-Pentadiene                | 223        | 39.4        | 3.99        | 275                                         | 0.248                           |
| 1,4-Pentadiene                    | 205        | 37.4        | 3.79        | 276                                         | 0.248                           |
| Pentafluorobenzene                | 258.9      | 34.7        | 3.52        |                                             |                                 |
| 2,3,4,5,6-Pentafluorotoluene      | 275.5      |             |             |                                             |                                 |
| 2,2,3,3,4-Pentamethyl-<br>pentane | 370.7      | 25.5        | 2.58        | 508                                         | 0.280                           |
| 2,2,3,4,4-Pentamethyl-<br>pentane | 354.2      | 23.7        | 2.40        | 521                                         | 0.273                           |
| Pentanal                          | 281        | 35          | 3.55        | 333                                         | 0.259                           |
| Pentane                           | 196.6      | 33.26       | 3.370       | 311                                         | 0.237                           |
| Pentanenitrile                    | 337.2      | 35.3        | 3.58        |                                             |                                 |
| Pentanethiol                      | 324.6      |             |             |                                             |                                 |
| Pentanoic acid                    | 370        | 35.3        | 3.58        | 340                                         | 0.300                           |
| 1-Pentanol                        | 315.0      | 38.38       | 3.889       | 326                                         | 0.270                           |
| 2-Pentanol                        | 287.3      | 36.27       | 3.675       |                                             |                                 |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                        | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|----------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 3-Pentanol                       | 286.5      |             |             |                                             |                                 |
| 2-Pentanone                      | 287.93     | 36.46       | 3.694       | 301                                         | 0.286                           |
| 3-Pentanone                      | 288.31     | 36.9        | 3.729       | 336                                         | 0.256                           |
| 1-Pentene                        | 191.63     | 34.81       | 3.527       | 293                                         | 0.239                           |
| <i>cis</i> -2-Pentene            | 202        | 36.4        | 3.69        |                                             |                                 |
| <i>trans</i> -2-Pentene          | 198        | 34.7        | 3.52        | 304                                         | 0.231                           |
| Pentyl acetate                   | 332        |             |             |                                             |                                 |
| Pentylbenzene                    | 406.8      | 25.7        | 2.60        | 550                                         | 0.269                           |
| Pentyl formate                   | 303        |             |             |                                             |                                 |
| 1-Pentyne                        | 220.3      | 40          | 4.05        | 278                                         | 0.245                           |
| Perchloryl fluoride              | 95.3       | 53.0        | 5.37        | 161                                         | 0.637                           |
| Phenanthrene                     | 596        |             |             | 554                                         | 0.322                           |
| Phenol                           | 421.1      | 60.5        | 6.13        | 229                                         | 0.41                            |
| 1-Phenylhexadecane               | 535        | 12.7        | 1.29        | 1200                                        | 0.252                           |
| 1-Phenylpentadecane              | 526.9      | 13.3        | 1.35        | 1140                                        | 0.253                           |
| 1-Phenyltetradecane              | 519        | 14.0        | 1.42        | 1110                                        | 0.247                           |
| Phosgene                         | 182        | 56          | 5.67        | 190                                         | 0.52                            |
| Phosphine                        | 51.3       | 64.5        | 6.54        |                                             |                                 |
| Phosphine- <i>d</i> <sub>3</sub> | 50.4       |             |             |                                             |                                 |
| Phosphonium chloride             | 49.1       | 72.7        | 7.37        |                                             |                                 |
| Phosphorus                       | 721        |             |             |                                             |                                 |
| Phosphorus bromide difluoride    | 113        |             |             |                                             |                                 |
| Phosphorus chloride difluoride   | 89.2       | 44.6        | 4.52        |                                             |                                 |
| Phosphorus dibromide fluoride    | 254        |             |             |                                             |                                 |
| Phosphorus dichloride fluoride   | 189.9      | 49.3        | 5.00        |                                             |                                 |
| Phosphorus pentachloride         | 372        |             |             |                                             |                                 |
| Phosphorus trichloride           | 290        |             |             | 260                                         | 0.528                           |
| Phosphorus trifluoride           | -1.9       | 42.7        | 4.33        |                                             |                                 |
| Phosphoryl chloride difluoride   | 150.7      | 43.4        | 4.40        |                                             |                                 |
| Phosphoryl trichloride           | 329        |             |             |                                             |                                 |
| Phosphoryl trifluoride           | 73.4       | 41.8        | 4.24        |                                             |                                 |
| Phthalic anhydride               | 537        | 47          | 4.76        | 368                                         | 0.402                           |
| Piperidine                       | 321.0      | 48.8        | 4.94        | 288                                         | 0.296                           |
| Propadiene                       | 120        | 54.0        | 5.47        | 162                                         | 0.247                           |
| Propanal                         | 231.3      | 52.0        | 5.27        | 204                                         | 0.285                           |
| Propane                          | 96.68      | 41.92       | 4.248       | 200                                         | 0.217                           |
| 1,2-Propanediol                  | 352        | 60          | 6.08        | 237                                         | 0.321                           |
| 1,3-Propanediol                  | 385        | 59          | 5.98        | 241                                         | 0.316                           |
| Propanenitrile                   | 288.2      | 42.0        | 4.26        | 230                                         | 0.240                           |
| 1-Propanethiol                   | 262.5      |             |             |                                             |                                 |
| 2-Propanethiol                   | 244.2      |             |             |                                             |                                 |
| Propanoic acid                   | 331        | 44.7        | 4.53        | 222                                         | 0.32                            |
| 1-Propanol                       | 263.7      | 51.01       | 5.169       | 218.5                                       | 0.275                           |
| 2-Propanol                       | 235.2      | 47.02       | 4.764       | 220                                         | 0.273                           |
| 2-Propenal                       | 233        | 51          | 5.17        | 197                                         | 0.285                           |
| Propene                          | 91.9       | 45.6        | 4.62        | 181                                         | 0.233                           |
| 2-Propen-1-ol                    | 272.0      |             |             | 208                                         | 0.279                           |
| Propyl acetate                   | 276.6      | 33.2        | 3.36        | 345                                         | 0.296                           |
| Propylamine                      | 223.9      | 46.6        | 4.72        | 233                                         | 0.254                           |
| Propylbenzene                    | 365.20     | 31.58       | 3.200       | 440                                         | 0.273                           |
| Propyl butanoate                 | 327        |             |             |                                             |                                 |
| Propylcyclopentane               | 358.7      | 29.6        | 3.00        | 425                                         | 0.264                           |
| Propylcyclohexane                | 336.7      | 27.7        | 2.81        |                                             |                                 |
| Propylene oxide                  | 209.1      | 48.6        | 4.92        | 186                                         | 0.312                           |

TABLE 6.5 Critical Properties (Continued)

| Substance                         | $T_c, ^\circ\text{C}$ | $P_c, \text{atm}$ | $P_c, \text{MPa}$ | $V_c, \text{cm}^3 \cdot \text{mol}^{-1}$ | $\rho_c, \text{g} \cdot \text{cm}^{-3}$ |
|-----------------------------------|-----------------------|-------------------|-------------------|------------------------------------------|-----------------------------------------|
| Propyl formate                    | 264.9                 | 40.1              | 4.06              | 285                                      | 0.309                                   |
| Propyl 2-methylpropanoate         | 316                   |                   |                   |                                          |                                         |
| Propyl 3-methylpropanoate         | 336                   |                   |                   |                                          |                                         |
| Propyl propanoate                 | 305                   |                   |                   |                                          |                                         |
| Propyne                           | 129.3                 | 55.5              | 5.62              | 164                                      | 0.245                                   |
| Pyridine                          | 346.9                 | 55.96             | 5.67              | 243                                      | 0.325                                   |
| Pyrrole                           | 366.6                 | 62.6              | 6.34              | 200                                      | 0.335                                   |
| Pyrrolidine                       | 295.1                 | 55.2              | 5.59              | 238                                      | 0.300                                   |
| Quinoline                         | 509                   | 48.0              | 4.86              | 437                                      | 0.300                                   |
| Radon                             | 104                   | 62                | 6.28              | 139                                      | 1.6                                     |
| Rhenium(VII) oxide                | 669                   |                   |                   | 334                                      |                                         |
| Rhenium(VI) oxide tetrachloride   | 508                   |                   |                   | 161                                      | 0.95                                    |
| Rubidium                          | 1832                  |                   |                   | 250                                      | 0.34                                    |
| Selenium                          | 1493                  |                   |                   |                                          |                                         |
| Silane                            | − 3.5                 | 47.8              | 4.84              |                                          |                                         |
| Silicon chloride trifluoride      | 34.5                  | 34.2              | 3.47              |                                          |                                         |
| Silicon tetrabromide              | 390                   |                   |                   |                                          |                                         |
| Silicon tetrachloride             | 234                   | 37                | 3.75              | 326                                      | 0.521                                   |
| Silicon tetrafluoride             | − 14.0                | 36.7              | 3.72              |                                          |                                         |
| Silicon trichloride fluoride      | 165.4                 | 35.3              | 3.57              |                                          |                                         |
| Spiro[2.2]pentane                 | 233.3                 |                   |                   |                                          |                                         |
| Styrene                           | 363.8                 | 36.3              | 3.68              | 347                                      | 0.300                                   |
| Sulfur                            | 1041                  | 116               | 11.7              |                                          |                                         |
| Sulfur dioxide                    | 157.7                 | 77.8              | 7.88              | 122                                      | 0.5240                                  |
| Sulfur hexafluoride               | 45.6                  | 37.1              | 3.76              | 198                                      | 0.734                                   |
| Sulfur tetrafluoride              | 91.7                  |                   |                   |                                          |                                         |
| Sulfur trioxide                   | 217.9                 | 81                | 8.2               | 130                                      | 0.633                                   |
| Tantalum pentabromide             | 701                   |                   |                   | 461                                      | 1.26                                    |
| Tantalum pentachloride            | 494                   |                   |                   | 400                                      | 0.89                                    |
| 1,2-Terphenyl                     | 617.9                 | 38.5              | 3.90              | 755                                      | 0.305                                   |
| 1,3-Terphenyl                     | 651.7                 | 34.6              | 3.51              | 768                                      | 0.300                                   |
| 1,4-Terphenyl                     | 652.9                 | 32.8              | 3.32              | 762                                      | 0.302                                   |
| 1,1,2,2-Tetrachlorodifluoroethane | 278                   | 34                | 3.44              | 371                                      | 0.549                                   |
| 1,1,2,2-Tetrachloroethane         | 388.00                |                   |                   |                                          |                                         |
| Tetrachloroethylene               | 347.1                 | 44.3              | 4.49              | 290                                      | 0.572                                   |
| Tetrachloromethane                | 283.5                 | 44.57             | 4.516             | 276                                      | 0.557                                   |
| Tetradecafluoro-1-heptene         | 205.1                 |                   |                   |                                          |                                         |
| Tetradecafluorohexane             | 174.5                 | 18.8              | 1.90              |                                          |                                         |
| Tetradecafluoromethylcyclohexane  | 213.7                 | 23                | 2.33              |                                          |                                         |
| Tetradecane                       | 420.9                 | 16                | 1.62              | 830                                      | 0.239                                   |
| 1-Tetradecene                     | 416                   | 15.4              | 1.56              |                                          |                                         |
| Tetradecylcyclopentane            | 499                   | 11.1              | 1.12              |                                          |                                         |
| Tetraethylsilane                  | 330.6                 | 25.68             | 2.602             |                                          |                                         |
| Tetrafluoroethylene               | 33.4                  | 38.9              | 3.91              | 175                                      | 0.58                                    |
| Tetrafluorohydrazine              | 33.3                  | 37                | 3.75              |                                          |                                         |
| Tetrafluoromethane                | − 45.5                | 36.9              | 3.74              | 140                                      | 0.629                                   |
| Tetrahydrofuran                   | 267.0                 | 51.22             | 5.19              | 224                                      | 0.322                                   |
| 1,2,3,4-Tetrahydronaphthalene     | 447                   | 36.0              | 3.65              | 408                                      | 0.324                                   |
| Tetrahydropyran                   | 299.1                 | 47.1              | 4.77              | 263                                      | 0.328                                   |
| Tetrahydrothiophene               | 358.9                 |                   |                   |                                          |                                         |
| 1,2,4,5-Tetramethylbenzene        | 402                   | 29                | 2.94              | 480                                      | 0.280                                   |
| 2,2,3,3-Tetramethylbutane         | 294.7                 | 28.3              | 2.87              | 461                                      | 0.248                                   |
| 2,2,3,3-Tetramethylhexane         | 350.0                 | 24.8              | 2.51              | 573                                      | 0.248                                   |

**TABLE 6.5** Critical Properties (*Continued*)

| Substance                                | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|------------------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 2,2,3,4-Tetramethylhexane                | 347.3      | 23.4        | 2.37        | 525                                         | 0.271                           |
| 2,2,3,5-Tetramethylhexane                | 328.2      | 22.4        | 2.27        | 540                                         | 0.263                           |
| 2,2,4,4-Tetramethylhexane                | 337.1      | 22.2        | 2.25        | 535                                         | 0.266                           |
| 2,2,4,5-Tetramethylhexane                | 325.4      | 21.9        | 2.22        | 544                                         | 0.262                           |
| 2,2,5,5-Tetramethylhexane                | 308.4      | 21.6        | 2.19        | 573                                         | 0.248                           |
| 2,3,3,4-Tetramethylhexane                | 360.0      | 24.5        | 2.48        | 514                                         | 0.277                           |
| 2,3,3,5-Tetramethylhexane                | 337.0      | 22.9        | 2.32        | 531                                         | 0.268                           |
| 2,3,4,4-Tetramethylhexane                | 353.5      | 23.9        | 2.42        | 518                                         | 0.275                           |
| 2,3,4,5-Tetramethylhexane                | 340.1      | 23.1        | 2.34        | 530                                         | 0.269                           |
| 3,3,4,4-Tetramethylhexane                | 373.6      | 25.4        | 2.57        | 506                                         | 0.281                           |
| 2,2,3,3-Tetramethylpentane               | 334.6      | 27.05       | 2.741       |                                             |                                 |
| 2,2,3,4-Tetramethylpentane               | 319.6      | 25.68       | 2.602       |                                             |                                 |
| 2,2,4,4-Tetramethylpentane               | 301.6      | 24.52       | 2.485       |                                             |                                 |
| 2,3,3,4-Tetramethylpentane               | 334.6      | 26.80       | 2.716       |                                             |                                 |
| Tetramethylsilane                        | 175.49     | 27.84       | 2.821       | 362                                         | 0.244                           |
| Thiacyclopentane                         | 358.8      |             |             |                                             |                                 |
| 2-Thiapropene                            | 230.0      | 54.6        | 5.53        | 201                                         | 0.309                           |
| Thiophene                                | 306.3      | 56.16       | 5.69        | 219                                         | 0.385                           |
| Thiophenol                               | 416.4      |             |             |                                             |                                 |
| Thymol                                   | 425        |             |             |                                             |                                 |
| Tin(IV) chloride                         | 318.7      | 37.0        | 3.75        | 351                                         | 0.742                           |
| Titanium tetrachloride                   | 365        | 46          | 4.66        | 340                                         | 0.558                           |
| Toluene                                  | 318.60     | 40.54       | 4.108       | 316                                         | 0.292                           |
| 1,2-Toluidine                            | 434        | 43.1        | 4.37        | 343                                         | 0.312                           |
| 1,3-Toluidine                            | 434        | 42.2        | 4.28        | 343                                         | 0.312                           |
| 1,4-Toluidine                            | 433        | 45.2        | 4.58        |                                             |                                 |
| Toluenitrile                             | 450        |             |             |                                             |                                 |
| Tributoxyborane                          | 472        | 19.6        | 1.99        | 863                                         | 0.267                           |
| Tributylamine                            | 365.3      | 18          | 1.82        |                                             |                                 |
| 1,1,1-Trichloroethane                    | 272        | 42.4        | 4.30        |                                             |                                 |
| 1,1,2-Trichloroethane                    | 329        | 41          | 4.15        | 294                                         | 0.454                           |
| Trichloroethylene                        | 271.1      | 49.5        | 5.02        | 256                                         | 0.513                           |
| Trichlorofluoromethane                   | 198.1      | 43.5        | 4.41        | 248                                         | 0.554                           |
| Trichlorofluorosilane                    | 165.4      | 35.3        | 3.57        |                                             |                                 |
| Trichloromethane                         | 263.3      | 54.0        | 5.47        | 239                                         | 0.500                           |
| Trichloromethylsilane                    | 244        | 32.4        | 3.28        | 348                                         | 0.430                           |
| 1,2,3-Trichloropropane                   | 378        | 39          | 3.95        | 348                                         | 0.424                           |
| 1,2,2-Trichlorotrifluoroethane           | 214.2      | 33.7        | 3.42        | 325                                         | 0.576                           |
| Tridecane                                | 402        | 16.6        | 1.68        | 780                                         | 0.236                           |
| 1-Tridecene                              | 401        | 16.8        | 1.70        |                                             |                                 |
| Tridecylcyclopentane                     | 488        | 11.9        | 1.21        |                                             |                                 |
| Triethanolamine                          | 514.3      | 24.2        | 2.45        |                                             |                                 |
| Triethylamine                            | 262.5      | 29.92       | 3.032       | 389                                         | 0.26                            |
| Trifluoroacetic acid                     | 218.2      | 32.15       | 3.258       | 204                                         | 0.559                           |
| Trifluoroamine oxide (NOF <sub>3</sub> ) | 29.5       |             |             | 169                                         | 0.593                           |
| 1,1,1-Trifluoroethane                    | 73.2       | 37.1        | 3.76        | 194                                         | 0.434                           |
| Trifluoromethane                         | 25.8       | 47.7        | 4.83        | 133                                         | 0.525                           |
| (Trifluoromethyl)benzene                 | 286.8      |             |             |                                             |                                 |
| Trimethylamine                           | 159.64     | 40.34       | 4.087       | 254                                         | 0.233                           |
| 1,2,3-Trimethylbenzene                   | 391.4      | 34.09       | 3.454       | 430                                         | 0.280                           |
| 1,2,4-Trimethylbenzene                   | 376.0      | 31.90       | 3.232       | 430                                         | 0.280                           |
| 1,3,5-Trimethylbenzene                   | 364.2      | 30.86       | 3.127       | 433                                         | 0.278                           |
| 2,2,3-Trimethylbutane                    | 258.1      | 29.15       | 2.954       | 398                                         | 0.252                           |
| 2,2,3-Trimethyl-1-butene                 | 260        | 28.6        | 2.90        | 400                                         | 0.245                           |

TABLE 6.5 Critical Properties (Continued)

| Substance                                              | $T_c$ , °C | $P_c$ , atm | $P_c$ , MPa | $V_c$ , cm <sup>3</sup> · mol <sup>-1</sup> | $\rho_c$ , g · cm <sup>-3</sup> |
|--------------------------------------------------------|------------|-------------|-------------|---------------------------------------------|---------------------------------|
| 1,1,2-Trimethylcyclopentane                            | 306.4      | 29.0        | 2.94        |                                             |                                 |
| 1,1,3-Trimethylcyclopentane                            | 296.4      | 27.9        | 2.83        |                                             |                                 |
| <i>cis,trans,cis</i> -1,2,4-Trimethyl-<br>cyclopentane | 298        | 27.7        | 2.81        |                                             |                                 |
| <i>cis,cis,trans</i> -1,2,4-Trimethyl-<br>cyclopentane | 306        | 28.4        | 2.88        |                                             |                                 |
| 2,2,3-Trimethylheptane                                 | 338.6      | 22.4        | 2.27        | 546                                         | 0.261                           |
| 2,2,4-Trimethylheptane                                 | 321.4      | 21.4        | 2.17        | 552                                         | 0.258                           |
| 2,2,5-Trimethylheptane                                 | 325.0      | 21.4        | 2.17        | 559                                         | 0.256                           |
| 2,2,6-Trimethylheptane                                 | 320.3      | 21.0        | 2.13        | 573                                         | 0.248                           |
| 2,3,3-Trimethylheptane                                 | 344.4      | 22.9        | 2.32        | 538                                         | 0.265                           |
| 2,3,4-Trimethylheptane                                 | 340.6      | 22.6        | 2.29        | 538                                         | 0.265                           |
| 2,3,5-Trimethylheptane                                 | 339.7      | 22.1        | 2.24        | 547                                         | 0.260                           |
| 2,3,6-Trimethylheptane                                 | 331.0      | 21.6        | 2.19        | 560                                         | 0.254                           |
| 2,4,4-Trimethylheptane                                 | 327.2      | 21.9        | 2.22        | 541                                         | 0.263                           |
| 2,4,5-Trimethylheptane                                 | 333.8      | 22.1        | 2.24        | 544                                         | 0.262                           |
| 2,4,6-Trimethylheptane                                 | 317.2      | 21.2        | 2.15        | 560                                         | 0.254                           |
| 2,5,5-Trimethylheptane                                 | 329.8      | 21.9        | 2.22        | 550                                         | 0.259                           |
| 3,3,4-Trimethylheptane                                 | 349.4      | 23.4        | 2.37        | 526                                         | 0.271                           |
| 3,3,5-Trimethylheptane                                 | 336.5      | 22.9        | 2.32        | 579                                         | 0.246                           |
| 3,4,4-Trimethylheptane                                 | 347.8      | 23.4        | 2.37        | 524                                         | 0.271                           |
| 3,4,5-Trimethylheptane                                 | 339.7      | 22.1        | 2.24        | 547                                         | 0.261                           |
| 2,2,3-Trimethylhexane                                  | 315        | 24.6        | 2.49        |                                             |                                 |
| 2,2,4-Trimethylhexane                                  | 300.6      | 23.4        | 2.37        |                                             |                                 |
| 2,2,5-Trimethylhexane                                  | 295        | 23.0        | 2.33        | 519                                         | 0.247                           |
| 2,4,7-Trimethyloctane                                  | 335.7      |             |             |                                             |                                 |
| 2,2,3-Trimethylpentane                                 | 290.4      | 26.94       | 2.730       | 436                                         | 0.262                           |
| 2,2,4-Trimethylpentane                                 | 270.9      | 25.34       | 2.568       | 468                                         | 0.244                           |
| 2,3,3-Trimethylpentane                                 | 300.5      | 27.83       | 2.820       | 455                                         | 0.251                           |
| 2,3,4-Trimethylpentane                                 | 293.4      | 26.94       | 2.730       | 461                                         | 0.248                           |
| 2,2,4-Trimethyl-1,3-pentanediol                        | 398        | 25.6        | 2.59        | 364.6                                       | 0.4010                          |
| 2,3,6-Trimethylpyridine                                | 381.4      |             |             |                                             |                                 |
| 2,4,6-Trimethylpyridine                                | 379.9      |             |             |                                             |                                 |
| 2,4,6-Trimethyl-1,3,5-trioxane                         | 290        |             |             |                                             |                                 |
| Tungsten(VI) oxide tetra-<br>chloride                  | 509        |             |             | 338                                         | 1.01                            |
| 1 <i>H</i> -Undecafluoropentane                        | 170.8      |             |             |                                             |                                 |
| Undecane                                               | 365.7      | 19.4        | 1.97        | 657                                         | 0.238                           |
| 1-Undecene                                             | 364        | 19.7        | 2.00        |                                             | 0.240                           |
| Uranium hexafluoride                                   | 232.7      | 45.5        | 4.61        | 250                                         | 1.41                            |
| Vinyl acetate                                          | 228.4      | 22.4        | 2.27        | 265                                         | 0.325                           |
| Vinyl chloride                                         | 156.6      | 55.3        | 5.60        | 169                                         | 0.370                           |
| Vinyl fluoride                                         | 54.7       | 51.7        | 5.24        | 114                                         | 0.320                           |
| Vinyl formate                                          | 202        | 57          | 5.78        | 210                                         | 0.343                           |
| Water                                                  | 374.2      | 217.6       | 22.04       | 56.0                                        | 0.325                           |
| Xenon                                                  | 16.583     | 57.64       | 5.84        | 118                                         | 1.105                           |
| 1,2-Xylene                                             | 357.2      | 36.83       | 3.732       | 370                                         | 0.288                           |
| 1,3-Xylene                                             | 343.9      | 34.95       | 3.541       | 375                                         | 0.282                           |
| 1,4-Xylene                                             | 343.1      | 34.65       | 3.511       | 379                                         | 0.280                           |
| Zirconium tetrabromide                                 | 532        |             |             | 415                                         | 0.99                            |
| Zirconium tetrachloride                                | 505        | 56.9        | 5.77        | 319                                         | 0.730                           |
| Zirconium tetraiodide                                  | 687        |             |             | 528                                         | 1.13                            |

# SECTION 7

---

## SPECTROSCOPY

---

|                                                                                                                                                                       |             |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|
| <b>7.1 X-RAY METHODS</b>                                                                                                                                              | <b>7.2</b>  |
| Table 7.1 Wavelengths of X-Ray Emission Spectra in Angstroms                                                                                                          | 7.3         |
| Table 7.2 Wavelengths of Absorption Edges in Angstroms                                                                                                                | 7.5         |
| Table 7.3 Critical X-Ray Absorption Energies in keV                                                                                                                   | 7.8         |
| Table 7.4 X-Ray Emission Energies in keV                                                                                                                              | 7.10        |
| Table 7.5 $\beta$ Filters for Common Target Elements                                                                                                                  | 7.14        |
| Table 7.6 Interplanar Spacings for $K\alpha_1$ Radiation, $d$ versus $2\theta$                                                                                        | 7.14        |
| Table 7.7 Analyzing Crystals for X-Ray Spectroscopy                                                                                                                   | 7.15        |
| Table 7.8 Mass Absorption Coefficients for $K\alpha_1$ Lines and $W L\alpha_1$ Line                                                                                   | 7.16        |
| <b>7.2 ULTRAVIOLET-VISIBLE SPECTROSCOPY</b>                                                                                                                           | <b>7.18</b> |
| Table 7.9 Electronic Absorption Bands for Representative Chromophores                                                                                                 | 7.19        |
| Table 7.10 Ultraviolet Cutoffs of Spectrograde Solvents                                                                                                               | 7.20        |
| Table 7.11 Absorption Wavelength of Dienes                                                                                                                            | 7.21        |
| Table 7.12 Absorption Wavelength of Enones and Dienones                                                                                                               | 7.22        |
| Table 7.13 Solvent Correction for Ultraviolet-Visible Spectroscopy                                                                                                    | 7.23        |
| Table 7.14 Primary Bands of Substituted Benzene and Heteroaromatics                                                                                                   | 7.23        |
| Table 7.15 Wavelength Calculation of the Principal Band of Substituted Benzene Derivatives                                                                            | 7.24        |
| <b>7.3 FLUORESCENCE</b>                                                                                                                                               | <b>7.25</b> |
| Table 7.16 Fluorescence Spectroscopy of Some Organic Compounds                                                                                                        | 7.25        |
| Table 7.17 Fluorescence Quantum Yield Values                                                                                                                          | 7.28        |
| <b>7.4 FLAME ATOMIC EMISSION, FLAME ATOMIC ABSORPTION, ELECTROTHERMAL (FURNACE) ATOMIC ABSORPTION, ARGON INDUCTION COUPLED PLASMA, AND PLASMA ATOMIC FLUORESCENCE</b> | <b>7.28</b> |
| Table 7.18 Detection Limits in ng/mL                                                                                                                                  | 7.29        |
| Table 7.19 Sensitive Lines of the Elements                                                                                                                            | 7.34        |
| 7.4.1 Some Common Spectroscopic Relationships                                                                                                                         | 7.38        |
| <b>7.5 INFRARED SPECTROSCOPY</b>                                                                                                                                      | <b>7.41</b> |
| Table 7.20 Absorption Frequencies of Single Bonds to Hydrogen                                                                                                         | 7.41        |
| Table 7.21 Absorption Frequencies of Triple Bonds                                                                                                                     | 7.47        |
| Table 7.22 Absorption Frequencies of Cumulated Double Bonds                                                                                                           | 7.49        |
| Table 7.23 Absorption Frequencies of Carbonyl Bands                                                                                                                   | 7.50        |
| 7.5.1 Intensities of Carbonyl Bands                                                                                                                                   | 7.53        |
| 7.5.2 Position of Carbonyl Absorption                                                                                                                                 | 7.53        |
| Table 7.24 Absorption Frequencies of Other Double Bonds                                                                                                               | 7.54        |
| Table 7.25 Absorption Frequencies of Aromatic Bands                                                                                                                   | 7.57        |
| Table 7.26 Absorption Frequencies of Miscellaneous Bands                                                                                                              | 7.58        |
| Table 7.27 Absorption Frequencies in the Near Infrared                                                                                                                | 7.64        |
| Table 7.28 Infrared Transmitting Materials                                                                                                                            | 7.67        |
| Table 7.29 Infrared Transmission Characteristics of Selected Solvents                                                                                                 | 7.68        |
| <b>7.6 RAMAN SPECTROSCOPY</b>                                                                                                                                         | <b>7.71</b> |
| Table 7.30 Raman Frequencies of Single Bonds to Hydrogen and Carbon                                                                                                   | 7.71        |
| Table 7.31 Raman Frequencies of Triple Bonds                                                                                                                          | 7.76        |
| Table 7.32 Raman Frequencies of Cumulated Double Bonds                                                                                                                | 7.77        |
| Table 7.33 Raman Frequencies of Carbonyl Bands                                                                                                                        | 7.78        |
| Table 7.34 Raman Frequencies of Other Double Bonds                                                                                                                    | 7.79        |
| Table 7.35 Raman Frequencies of Aromatic Compounds                                                                                                                    | 7.82        |
| Table 7.36 Raman Frequencies of Sulfur Compounds                                                                                                                      | 7.84        |
| Table 7.37 Raman Frequencies of Ethers                                                                                                                                | 7.85        |



|            |                                                                                       |       |
|------------|---------------------------------------------------------------------------------------|-------|
| Table 7.38 | Raman Frequencies of Halogen Compounds                                                | 7.86  |
| Table 7.39 | Raman Frequencies of Miscellaneous Compounds                                          | 7.87  |
| Table 7.40 | Principal Argon-Ion Laser Plasma Lines                                                | 7.88  |
| 7.7        | NUCLEAR MAGNETIC RESONANCE                                                            | 7.89  |
| Table 7.41 | Nuclear Properties of the Elements                                                    | 7.89  |
| Table 7.42 | Proton Chemical Shifts                                                                | 7.92  |
| Table 7.43 | Estimation of Chemical Shift for Protons of $\text{—CH}_2\text{—}$ and Methine Groups | 7.94  |
| Table 7.44 | Estimation of Chemical Shift of Proton Attached to a Double Bond                      | 7.95  |
| Table 7.45 | Chemical Shifts in Monosubstituted Benzene                                            | 7.96  |
| Table 7.46 | Proton Spin Coupling Constants                                                        | 7.97  |
| Table 7.47 | Proton Chemical Shifts of Reference Compounds                                         | 7.98  |
| Table 7.48 | Solvent Positions of Residual Protons in Incompletely Deuterated Solvents             | 7.98  |
| Table 7.49 | Carbon-13 Chemical Shifts                                                             | 7.99  |
| Table 7.50 | Estimation of Chemical Shifts of Alkane Carbons                                       | 7.102 |
| Table 7.51 | Effect of Substituent Groups on Alkyl Chemical Shifts                                 | 7.102 |
| Table 7.52 | Estimation of Chemical Shifts of Carbon Attached to a Double Bond                     | 7.103 |
| Table 7.53 | Carbon-13 Chemical Shifts in Substituted Benzenes                                     | 7.104 |
| Table 7.54 | Carbon-13 Chemical Shifts in Substituted Pyridines                                    | 7.105 |
| Table 7.55 | Carbon-13 Chemical Shifts of Carbonyl Group                                           | 7.106 |
| Table 7.56 | One-Bond Carbon-Hydrogen Spin Coupling Constants                                      | 7.107 |
| Table 7.57 | Two-Bond Carbon-Hydrogen Spin Coupling Constants                                      | 7.108 |
| Table 7.58 | Carbon-Carbon Spin Coupling Constants                                                 | 7.108 |
| Table 7.59 | Carbon-Fluorine Spin Coupling Constants                                               | 7.109 |
| Table 7.60 | Carbon-13 Chemical Shifts of Deuterated Solvents                                      | 7.110 |
| Table 7.61 | Carbon-13 Coupling Constants with Various Nuclei                                      | 7.110 |
| Table 7.62 | Boron-11 Chemical Shifts                                                              | 7.111 |
| Table 7.63 | Nitrogen-15 (or Nitrogen-14) Chemical Shifts                                          | 7.112 |
| Table 7.64 | Nitrogen-15 Chemical Shifts in Monosubstituted Pyridine                               | 7.115 |
| Table 7.65 | Nitrogen-15 Chemical Shifts for Standards                                             | 7.115 |
| Table 7.66 | Nitrogen-15 to Hydrogen-1 Spin Coupling Constants                                     | 7.115 |
| Table 7.67 | Nitrogen-15 to Carbon-13 Spin Coupling Constants                                      | 7.116 |
| Table 7.68 | Nitrogen-15 to Fluorine-19 Spin Coupling Constants                                    | 7.116 |
| Table 7.69 | Fluorine-19 Chemical Shifts                                                           | 7.117 |
| Table 7.70 | Fluorine-19 Chemical Shifts for Standards                                             | 7.118 |
| Table 7.71 | Fluorine-19 to Fluorine-19 Spin Coupling Constants                                    | 7.118 |
| Table 7.72 | Silicon-29 Chemical Shifts                                                            | 7.118 |
| Table 7.73 | Phosphorus-31 Chemical Shifts                                                         | 7.119 |
| Table 7.74 | Phosphorus-31 Spin Coupling Constants                                                 | 7.122 |
| 7.8        | MASS SPECTROMETRY                                                                     | 7.123 |
| 7.8.1      | Correlation of Mass Spectra with Molecular Structure                                  | 7.123 |
| Table 7.75 | Isotopic Abundances and Masses of Selected Elements                                   | 7.124 |
| 7.8.2      | Mass Spectra and Structure                                                            | 7.126 |
| Table 7.76 | Condensed Table of Mass Spectra                                                       | 7.128 |

## 7.1 X-RAY METHODS

An X-ray tube operating at a voltage  $V$  (in keV) emits a continuous X-ray spectrum, the minimum wavelength of which is given by  $\lambda_{\min} = 12.398/V$  with the wavelength expressed in angstroms. For expressing the wavelength in  $kX$  units, divide by the factor 1.00202. Tables 7.1 and 7.2 are based

**TABLE 7.1** Wavelengths of X-Ray Emission Spectra in Angstroms

| Atomic No. | Element | $K\alpha_2$ | $K\alpha_1$ | $K\beta_1$ | $L\alpha_1$ | $L\beta_1$ |
|------------|---------|-------------|-------------|------------|-------------|------------|
| 3          | Li      | 240         |             |            |             |            |
| 4          | Be      | 113         |             |            |             |            |
| 5          | B       | 67          |             |            |             |            |
| 6          | C       | 44          |             |            |             |            |
| 7          | N       | 31.60       |             |            |             |            |
| 8          | O       | 23.71       |             |            |             |            |
| 9          | F       | 18.31       |             |            |             |            |
| 10         | Ne      | 14.616      |             | 14.464     |             |            |
| 11         | Na      | 11.909      |             | 11.617     | 407.6       |            |
| 12         | Mg      | 9.889       |             | 9.558      | 251.0       |            |
| 13         | Al      | 8.3392      | 8.3367      | 7.981      | 169.8       |            |
| 14         | Si      | 7.1277      | 7.1253      | 6.7681     | 123         |            |
| 15         | P       | 6.1549      |             | 5.8038     |             |            |
| 16         | S       | 5.3747      | 5.3720      | 5.0317     |             |            |
| 17         | Cl      | 4.7305      | 4.7276      | 4.4031     |             |            |
| 18         | Ar      | 4.1946      | 4.1916      | 3.8848     |             |            |
| 19         | K       | 3.7446      | 3.7412      | 3.4538     | 42.7        |            |
| 20         | Ca      | 3.3616      | 3.3583      | 3.0896     | 36.32       | 35.95      |
| 21         | Sc      | 3.0345      | 3.0311      | 2.7795     | 31.33       | 31.01      |
| 22         | Ti      | 2.75207     | 2.7484      | 2.5138     | 27.39       | 27.02      |
| 23         | V       | 2.5073      | 2.5035      | 2.2843     | 24.26       | 23.85      |
| 24         | Cr      | 2.29351     | 2.28962     | 2.08480    | 21.67       | 21.28      |
| 25         | Mn      | 2.1057      | 2.1018      | 1.9102     | 19.45       | 19.12      |
| 26         | Fe      | 1.93991     | 1.93597     | 1.75653    | 17.567      | 17.255     |
| 27         | Co      | 1.79278     | 1.78892     | 1.62075    | 15.968      | 15.667     |
| 28         | Ni      | 1.66169     | 1.65784     | 1.50010    | 14.566      | 14.279     |
| 29         | Cu      | 1.54433     | 1.54051     | 1.39217    | 13.330      | 13.053     |
| 30         | Zn      | 1.4389      | 1.4351      | 1.2952     | 12.257      | 11.985     |
| 31         | Ga      | 1.3439      | 1.3400      | 1.20784    | 11.290      | 11.023     |
| 32         | Ge      | 1.2580      | 1.2540      | 1.1289     | 10.435      | 10.174     |
| 33         | As      | 1.1798      | 1.1758      | 1.0573     | 9.671       | 9.414      |
| 34         | Se      | 1.1088      | 1.1047      | 0.9921     | 8.990       | 8.736      |
| 35         | Br      | 1.0438      | 1.0397      | 0.9327     | 8.375       | 8.125      |
| 36         | Kr      | 0.9841      | 0.9801      | 0.8785     | 7.822       | 7.574      |
| 37         | Rb      | 0.9296      | 0.9255      | 0.8286     | 7.3181      | 7.076      |
| 38         | Sr      | 0.8794      | 0.8752      | 0.7829     | 6.8625      | 6.6237     |
| 39         | Y       | 0.8330      | 0.8279      | 0.7407     | 6.4485      | 6.2117     |
| 40         | Zr      | 0.7901      | 0.7859      | 0.7017     | 6.0702      | 5.8358     |
| 41         | Nb      | 0.7504      | 0.7462      | 0.6657     | 5.7240      | 5.4921     |
| 42         | Mo      | 0.713543    | 0.70926     | 0.632253   | 5.4063      | 5.1768     |
| 43         | Tc      | 0.6793      | 0.6749      | 0.6014     | 5.1126      | 4.8782     |
| 44         | Ru      | 0.6474      | 0.6430      | 0.5725     | 4.8455      | 4.6204     |
| 45         | Rh      | 0.6176      | 0.6132      | 0.5456     | 4.5973      | 4.3739     |

**TABLE 7.1** Wavelengths of X-Ray Emission Spectra in Angstroms (*Continued*)

| Atomic No. | Element | $K\alpha_2$ | $K\alpha_1$ | $K\beta_1$ | $L\alpha_1$ | $L\beta_1$ |
|------------|---------|-------------|-------------|------------|-------------|------------|
| 46         | Pd      | 0.5898      | 0.5854      | 0.5205     | 4.3676      | 4.1460     |
| 47         | Ag      | 0.563775    | 0.559363    | 0.49701    | 4.1541      | 3.9344     |
| 48         | Cd      | 0.5394      | 0.5350      | 0.4751     | 3.9563      | 3.7381     |
| 49         | In      | 0.5165      | 0.5121      | 0.4545     | 3.7719      | 3.5552     |
| 50         | Sn      | 0.4950      | 0.4906      | 0.4352     | 3.5999      | 3.3848     |
| 51         | Sb      | 0.4748      | 0.4703      | 0.4171     | 3.4392      | 3.2256     |
| 52         | Te      | 0.4558      | 0.4513      | 0.4000     | 3.2891      | 3.0767     |
| 53         | I       | 0.4378      | 0.4333      | 0.3839     | 3.1485      | 2.9373     |
| 54         | Xe      | 0.4204      | 0.4160      | 0.3685     | 3.016       | 2.807      |
| 55         | Cs      | 0.4048      | 0.4003      | 0.3543     | 2.9016      | 2.8920     |
| 56         | Ba      | 0.3896      | 0.3851      | 0.3408     | 2.7752      | 2.5674     |
| 57         | La      | 0.3753      | 0.3707      | 0.3280     | 2.6651      | 2.4583     |
| 58         | Ce      | 0.3617      | 0.3571      | 0.3158     | 2.5612      | 2.3558     |
| 59         | Pr      | 0.3487      | 0.3441      | 0.3042     | 2.4627      | 2.2584     |
| 60         | Nd      | 0.3565      | 0.3318      | 0.2933     | 2.3701      | 2.1666     |
| 61         | Pm      | 0.3249      | 0.3207      | 0.2821     | 2.282       | 2.0796     |
| 62         | Sm      | 0.3137      | 0.3190      | 0.2731     | 2.1994      | 1.9976     |
| 63         | Eu      | 0.3133      | 0.2985      | 0.2636     | 2.1206      | 1.9202     |
| 64         | Gd      | 0.2932      | 0.2884      | 0.2544     | 2.0460      | 1.8462     |
| 65         | Tb      | 0.2834      | 0.2788      | 0.2460     | 1.9755      | 1.7763     |
| 66         | Dy      | 0.2743      | 0.2696      | 0.2376     | 1.9088      | 1.7100     |
| 67         | Ho      | 0.2655      | 0.2608      | 0.2302     | 1.8447      | 1.6468     |
| 68         | Er      | 0.2572      | 0.2525      | 0.2226     | 1.7843      | 1.5873     |
| 69         | Tm      | 0.2491      | 0.2444      | 0.2153     | 1.7263      | 1.5299     |
| 70         | Yb      | 0.2415      | 0.2368      | 0.2088     | 1.6719      | 1.4756     |
| 71         | Lu      | 0.2341      | 0.2293      | 0.2021     | 1.6194      | 1.4235     |
| 72         | Hf      | 0.2270      | 0.2222      | 0.1955     | 1.5696      | 1.3740     |
| 73         | Ta      | 0.2203      | 0.2155      | 0.1901     | 1.5219      | 1.3270     |
| 74         | W       | 0.213813    | 0.208992    | 0.184363   | 1.4764      | 1.2818     |
| 75         | Re      | 0.2076      | 0.2028      | 0.1789     | 1.4329      | 1.2385     |
| 76         | Os      | 0.2016      | 0.1968      | 0.1736     | 1.3911      | 1.1972     |
| 77         | Ir      | 0.1959      | 0.1910      | 0.1685     | 1.3513      | 1.1578     |
| 78         | Pt      | 0.1904      | 0.1855      | 0.1637     | 1.3130      | 1.1198     |
| 79         | Au      | 0.1851      | 0.1802      | 0.1590     | 1.2764      | 1.0836     |
| 80         | Hg      | 0.1799      | 0.1750      | 0.1544     | 1.2411      | 1.0486     |
| 81         | Tl      | 0.1750      | 0.1701      | 0.1501     | 1.2074      | 1.0152     |
| 82         | Pb      | 0.1703      | 0.1654      | 0.1460     | 1.1750      | 0.9822     |
| 83         | Bi      | 0.1657      | 0.1608      | 0.1419     | 1.1439      | 0.9520     |
| 84         | Po      | 0.1608      | 0.1559      | 0.1382     | 1.1138      | 0.9222     |
| 85         | At      | 0.1570      | 0.1521      | 0.1343     | 1.0850      | 0.8936     |
| 86         | Rn      | 0.1529      | 0.1479      | 0.1307     | 1.0572      | 0.8659     |
| 87         | Fr      | 0.1489      | 0.1440      | 0.1272     | 1.030       | 0.840      |
| 88         | Ra      | 0.1450      | 0.1401      | 0.1237     | 1.0047      | 0.8137     |
| 89         | Ac      | 0.1414      | 0.1364      | 0.1205     | 0.9799      | 0.7890     |
| 90         | Th      | 0.1378      | 0.1328      | 0.1174     | 0.9560      | 0.7652     |

**TABLE 7.1** Wavelengths of X-Ray Emission Spectra in Angstroms (*Continued*)

| Atomic No. | Element | $K\alpha_2$ | $K\alpha_1$ | $K\beta_1$ | $L\alpha_1$ | $L\beta_1$ |
|------------|---------|-------------|-------------|------------|-------------|------------|
| 91         | Pa      | 0.1344      | 0.1294      | 0.1143     | 0.9328      | 0.7422     |
| 92         | U       | 0.1310      | 0.1259      | 0.1114     | 0.9105      | 0.7200     |
| 93         | Np      | 0.1278      | 0.1226      | 0.1085     | 0.8893      | 0.6984     |
| 94         | Pu      | 0.1246      | 0.1195      | 0.1058     | 0.8682      | 0.6777     |
| 95         | Am      | 0.1215      | 0.1165      | 0.1031     | 0.8481      | 0.6576     |
| 96         | Cm      | 0.1186      | 0.1135      | 0.1005     | 0.8287      | 0.6388     |
| 97         | Bk      | 0.1157      | 0.1107      | 0.0980     | 0.8098      | 0.6203     |
| 98         | Cf      | 0.1130      | 0.1079      | 0.0956     | 0.7917      | 0.6023     |
| 99         | Es      | 0.1103      | 0.1052      | 0.0933     | 0.7740      | 0.5850     |
| 100        | Fm      | 0.1077      | 0.1026      | 0.0910     | 0.7570      | 0.5682     |

**TABLE 7.2** Wavelengths of Absorption Edges in Angstroms

| Atomic No. | Element | $K$     | $L_I$ | $L_{II}$ | $L_{III}$ |
|------------|---------|---------|-------|----------|-----------|
| 3          | Li      | 226.5   |       |          |           |
| 4          | Be      | 110.68  |       |          |           |
| 5          | B       | 66.289  |       |          |           |
| 6          | C       | 43.68   |       |          |           |
| 7          | N       | 30.99   |       |          |           |
| 8          | O       | 23.32   |       |          |           |
| 9          | F       | 17.913  |       |          |           |
| 10         | Ne      | 14.183  |       |          |           |
| 11         | Na      | 11.478  |       | 400      |           |
| 12         | Mg      | 9.512   | 197.4 | 247.92   |           |
| 13         | Al      | 7.951   | 142.5 | 170      |           |
| 14         | Si      | 6.745   | 105.1 | 126.48   |           |
| 15         | P       | 5.787   | 81.0  | 96.84    |           |
| 16         | S       | 5.018   | 64.23 | 76.05    |           |
| 17         | Cl      | 4.397   | 52.08 | 61.37    | 62.93     |
| 18         | Ar      | 3.871   | 43.19 | 50.39    | 50.60     |
| 19         | K       | 3.436   | 36.35 | 42.02    | 42.17     |
| 20         | Ca      | 3.070   | 31.07 | 35.20    | 35.49     |
| 21         | Sc      | 2.757   | 26.83 | 30.16    | 30.53     |
| 22         | Ti      | 2.497   | 23.39 | 26.83    | 27.37     |
| 23         | V       | 2.269   | 20.52 | 23.70    | 24.26     |
| 24         | Cr      | 2.07012 | 16.7  | 17.9     | 20.7      |
| 25         | Mn      | 1.896   | 16.27 | 18.90    | 19.40     |
| 26         | Fe      | 1.74334 | 14.60 | 17.17    | 17.53     |
| 27         | Co      | 1.60811 | 13.34 | 15.53    | 15.93     |
| 28         | Ni      | 1.48802 | 12.27 | 14.13    | 14.58     |
| 29         | Cu      | 1.38043 | 11.27 | 13.01    | 13.29     |
| 30         | Zn      | 1.283   | 10.33 | 11.86    | 12.13     |

**TABLE 7.2** Wavelengths of Absorption Edges in Angstroms (*Continued*)

| Atomic No. | Element | $K$     | $L_I$ | $L_{II}$ | $L_{III}$ |
|------------|---------|---------|-------|----------|-----------|
| 31         | Ga      | 1.195   | 9.54  | 10.61    | 11.15     |
| 32         | Ge      | 1.116   | 8.73  | 9.97     | 10.23     |
| 33         | As      | 1.044   | 8.108 | 9.124    | 9.367     |
| 34         | Se      | 0.9800  | 7.505 | 8.417    | 8.646     |
| 35         | Br      | 0.9199  | 6.925 | 7.752    | 7.989     |
| 36         | Kr      | 0.8655  | 6.456 | 7.165    | 7.395     |
| 37         | Rb      | 0.8155  | 5.997 | 6.643    | 6.863     |
| 38         | Sr      | 0.7697  | 5.582 | 6.172    | 6.387     |
| 39         | Y       | 0.7276  | 5.233 | 5.756    | 5.962     |
| 40         | Zr      | 0.6888  | 4.867 | 5.378    | 5.583     |
| 41         | Nb      | 0.6529  | 4.581 | 5.025    | 5.223     |
| 42         | Mo      | 0.61977 | 4.299 | 4.719    | 4.912     |
| 43         | Tc      | 0.5888  | 4.064 | 4.427    | 4.629     |
| 44         | Ru      | 0.5605  | 3.841 | 4.179    | 4.369     |
| 45         | Rh      | 0.5338  | 3.626 | 3.942    | 4.130     |
| 46         | Pd      | 0.5092  | 3.428 | 3.724    | 3.908     |
| 47         | Ag      | 0.48582 | 3.254 | 3.514    | 3.698     |
| 48         | Cd      | 0.4641  | 3.084 | 3.326    | 3.504     |
| 49         | In      | 0.4439  | 2.926 | 3.147    | 3.324     |
| 50         | Sn      | 0.4247  | 2.778 | 2.982    | 3.156     |
| 51         | Sb      | 0.4066  | 2.639 | 2.830    | 3.000     |
| 52         | Te      | 0.3897  | 2.510 | 2.687    | 2.855     |
| 53         | I       | 0.3738  | 2.390 | 2.553    | 2.719     |
| 54         | Xe      | 0.3585  | 2.274 | 2.429    | 2.592     |
| 55         | Cs      | 0.3447  | 2.167 | 2.314    | 2.474     |
| 56         | Ba      | 0.3314  | 2.068 | 2.204    | 2.363     |
| 57         | La      | 0.3184  | 1.973 | 2.103    | 2.258     |
| 58         | Ce      | 0.3065  | 1.891 | 2.009    | 2.164     |
| 59         | Pr      | 0.2952  | 1.811 | 1.924    | 2.077     |
| 60         | Nd      | 0.2845  | 1.735 | 1.843    | 1.995     |
| 61         | Pm      | 0.2743  | 1.668 | 1.766    | 1.918     |
| 62         | Sm      | 0.2646  | 1.598 | 1.702    | 1.845     |
| 63         | Eu      | 0.2555  | 1.536 | 1.626    | 1.775     |
| 64         | Gd      | 0.2468  | 1.477 | 1.561    | 1.709     |
| 65         | Tb      | 0.2384  | 1.421 | 1.501    | 1.649     |
| 66         | Dy      | 0.2305  | 1.365 | 1.438    | 1.579     |
| 67         | Ho      | 0.2229  | 1.319 | 1.390    | 1.535     |
| 68         | Er      | 0.2157  | 1.269 | 1.339    | 1.483     |
| 69         | Tm      | 0.2089  | 1.222 | 1.288    | 1.433     |
| 70         | Yb      | 0.2022  | 1.181 | 1.243    | 1.386     |
| 71         | Lu      | 0.1958  | 1.140 | 1.198    | 1.341     |
| 72         | Hf      | 0.1898  | 1.099 | 1.154    | 1.297     |
| 73         | Ta      | 0.1839  | 1.061 | 1.113    | 1.255     |

**TABLE 7.2** Wavelengths of Absorption Edges in Angstroms (*Continued*)

| Atomic No. | Element | $K$     | $L_I$  | $L_{II}$ | $L_{III}$ |
|------------|---------|---------|--------|----------|-----------|
| 74         | W       | 0.17837 | 1.025  | 1.074    | 1.215     |
| 75         | Re      | 0.1731  | 0.9901 | 1.036    | 1.177     |
| 76         | Os      | 0.1678  | 0.9557 | 1.001    | 1.140     |
| 77         | Ir      | 0.1629  | 0.9243 | 0.9670   | 1.106     |
| 78         | Pt      | 0.1582  | 0.8914 | 0.9348   | 1.072     |
| 79         | Au      | 0.1534  | 0.8638 | 0.9028   | 1.040     |
| 80         | Hg      | 0.1492  | 0.8353 | 0.8779   | 1.009     |
| 81         | Tl      | 0.1447  | 0.8079 | 0.8436   | 0.9793    |
| 82         | Pb      | 0.1408  | 0.7815 | 0.8155   | 0.9503    |
| 83         | Bi      | 0.1371  | 0.7565 | 0.7891   | 0.9234    |
| 84         | Po      | 0.1332  | 0.7322 | 0.7638   | 0.8970    |
| 85         | At      | 0.1295  | 0.7092 | 0.7387   | 0.8720    |
| 86         | Rn      | 0.1260  | 0.6868 | 0.7153   | 0.8479    |
| 87         | Fr      | 0.1225  | 0.6654 | 0.6929   | 0.8248    |
| 88         | Ra      | 0.1192  | 0.6446 | 0.6711   | 0.8027    |
| 89         | Ac      | 0.1161  | 0.6248 | 0.6500   | 0.7813    |
| 90         | Th      | 0.1129  | 0.6061 | 0.6301   | 0.7606    |
| 91         | Pa      | 0.1101  | 0.5875 | 0.6106   | 0.7411    |
| 92         | U       | 0.1068  | 0.5697 | 0.5919   | 0.7233    |
| 93         | Np      | 0.1045  | 0.5531 | 0.5742   | 0.7042    |
| 94         | Pu      | 0.1018  | 0.5366 | 0.5571   | 0.6867    |
| 95         | Am      | 0.0992  | 0.5208 | 0.5404   | 0.6700    |
| 96         | Cm      | 0.0967  | 0.5060 | 0.5246   | 0.6532    |
| 97         | Bk      | 0.0943  | 0.4913 | 0.5093   | 0.6375    |
| 98         | Cf      | 0.0920  | 0.4771 | 0.4945   | 0.6223    |
| 99         | Es      | 0.0897  | 0.4636 | 0.4801   | 0.6076    |
| 100        | Fm      | 0.0875  | 0.4506 | 0.4665   | 0.5935    |

on the  $K$  and  $L$  wavelength values as published by Y. Cauchois and H. Hulubei (*Tables de Constantes et Données Numériques, I. Longueurs d'Onde des Émissions X et des Discontinuités d'Absorption X*, Hermann, Paris, 1947) and by the International Union of Crystallography (*International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham, England, 1962). Wavelength accuracy is only to about 1 in 25 000 except for the lines employed in X-ray diffraction work.

Use of energy-proportional detectors for X-rays creates a need for energy values of  $K$  and  $L$  absorption edges (Table 7.3) and emission series (Table 7.4). These values were obtained by a conversion to keV of tabulated experimental wavelength values and smoothed by a fit to Moseley's law. Although values are listed to 1 eV, chemical form may shift absorption edges and emission lines as much as 10 to 20 eV. S. Fine and C. F. Hendee [*Nuclonics*, **13**(3):36 (1955)] also give values for  $K\beta_2$ ,  $L\gamma_1$ , and  $L\beta_2$  lines.

The relative intensities of X-ray emission lines from targets varies for different elements. However, one can assume a ratio of  $K\alpha_1/K\alpha_2 = 2$  for the commonly used targets. The ratio of  $K\alpha_2/K\beta_1$  from these targets varies from 6 to 3.5. The intensities of  $K\beta_2$  radiations amount to about 1 percent

**TABLE 7.3** Critical X-Ray Absorption Energies in keV

| Atomic No. | Element | $K$    | $L_I$  | $L_{II}$ | $L_{III}$ |
|------------|---------|--------|--------|----------|-----------|
| 1          | H       | 0.0136 |        |          |           |
| 2          | He      | 0.0246 |        |          |           |
| 3          | Li      | 0.0547 |        |          |           |
| 4          | Be      | 0.112  |        |          |           |
| 5          | B       | 0.187  |        |          |           |
| 6          | C       | 0.284  |        |          |           |
| 7          | N       | 0.400  |        |          |           |
| 8          | O       | 0.532  |        |          |           |
| 9          | F       | 0.692  |        |          |           |
| 10         | Ne      | 0.874  | 0.048  | 0.022    |           |
| 11         | Na      | 1.08   | 0.055  | 0.034    |           |
| 12         | Mg      | 1.30   | 0.0628 | 0.0502   |           |
| 13         | Al      | 1.559  | 0.0870 | 0.0720   |           |
| 14         | Si      | 1.838  | 0.118  | 0.0977   |           |
| 15         | P       | 2.142  | 0.153  | 0.128    |           |
| 16         | S       | 2.469  | 0.193  | 0.163    | 0.162     |
| 17         | Cl      | 2.822  | 0.238  | 0.202    | 0.201     |
| 18         | Ar      | 3.200  | 0.287  | 0.246    | 0.244     |
| 19         | K       | 3.606  | 0.341  | 0.295    | 0.292     |
| 20         | Ca      | 4.038  | 0.399  | 0.350    | 0.346     |
| 21         | Sc      | 4.496  | 0.462  | 0.411    | 0.407     |
| 22         | Ti      | 4.966  | 0.530  | 0.462    | 0.456     |
| 23         | V       | 5.467  | 0.604  | 0.523    | 0.515     |
| 24         | Cr      | 5.988  | 0.679  | 0.584    | 0.574     |
| 25         | Mn      | 6.542  | 0.762  | 0.656    | 0.644     |
| 26         | Fe      | 7.113  | 0.849  | 0.722    | 0.709     |
| 27         | Co      | 7.713  | 0.929  | 0.798    | 0.783     |
| 28         | Ni      | 8.337  | 1.02   | 0.877    | 0.858     |
| 29         | Cu      | 8.982  | 1.10   | 0.954    | 0.935     |
| 30         | Zn      | 9.662  | 1.20   | 1.05     | 1.02      |
| 31         | Ga      | 10.39  | 1.30   | 1.17     | 1.14      |
| 32         | Ge      | 11.10  | 1.42   | 1.24     | 1.21      |
| 33         | As      | 11.87  | 1.529  | 1.358    | 1.32      |
| 34         | Se      | 12.65  | 1.66   | 1.472    | 1.431     |
| 35         | Br      | 13.48  | 1.791  | 1.599    | 1.552     |
| 36         | Kr      | 14.32  | 1.92   | 1.729    | 1.674     |
| 37         | Rb      | 15.197 | 2.064  | 1.863    | 1.803     |
| 38         | Sr      | 16.101 | 2.212  | 2.004    | 1.937     |
| 39         | Y       | 17.053 | 2.387  | 2.171    | 2.096     |
| 40         | Zr      | 17.998 | 2.533  | 2.308    | 2.224     |
| 41         | Nb      | 18.986 | 2.700  | 2.467    | 2.372     |
| 42         | Mo      | 20.003 | 2.869  | 2.630    | 2.525     |
| 43         | Tc      | 21.050 | 3.045  | 2.796    | 2.680     |

**TABLE 7.3** Critical X-Ray Absorption Energies in keV (*Continued*)

| Atomic No. | Element | $K$    | $L_I$  | $L_{II}$ | $L_{III}$ |
|------------|---------|--------|--------|----------|-----------|
| 44         | Ru      | 22.117 | 3.227  | 2.968    | 2.839     |
| 45         | Rh      | 23.210 | 3.404  | 3.139    | 2.995     |
| 46         | Pd      | 24.356 | 3.614  | 3.338    | 3.181     |
| 47         | Ag      | 25.535 | 3.828  | 3.547    | 3.375     |
| 48         | Cd      | 26.712 | 4.019  | 3.731    | 3.541     |
| 49         | In      | 27.929 | 4.226  | 3.929    | 3.732     |
| 50         | Sn      | 29.182 | 4.445  | 4.139    | 3.911     |
| 51         | Sb      | 30.497 | 4.708  | 4.391    | 4.137     |
| 52         | Te      | 31.817 | 4.953  | 4.621    | 4.347     |
| 53         | I       | 33.164 | 5.187  | 4.855    | 4.559     |
| 54         | Xe      | 34.551 | 5.448  | 5.103    | 4.783     |
| 55         | Cs      | 35.974 | 5.706  | 5.360    | 5.014     |
| 56         | Ba      | 37.432 | 5.995  | 5.629    | 5.250     |
| 57         | La      | 38.923 | 6.264  | 5.902    | 5.490     |
| 58         | Ce      | 40.43  | 6.556  | 6.169    | 5.728     |
| 59         | Pr      | 41.99  | 6.837  | 6.446    | 5.968     |
| 60         | Nd      | 43.57  | 7.134  | 6.728    | 6.215     |
| 61         | Pm      | 45.19  | 7.431  | 7.022    | 6.462     |
| 62         | Sm      | 46.85  | 7.742  | 7.316    | 6.720     |
| 63         | Eu      | 48.51  | 8.059  | 7.624    | 6.984     |
| 64         | Gd      | 50.23  | 8.383  | 7.942    | 7.251     |
| 65         | Tb      | 52.00  | 8.713  | 8.258    | 7.520     |
| 66         | Dy      | 53.77  | 9.053  | 8.587    | 7.795     |
| 67         | Ho      | 55.61  | 9.395  | 8.918    | 8.074     |
| 68         | Er      | 57.47  | 9.754  | 9.270    | 8.362     |
| 69         | Tm      | 59.38  | 10.12  | 9.622    | 8.656     |
| 70         | Yb      | 61.31  | 10.49  | 9.985    | 8.949     |
| 71         | Lu      | 63.32  | 10.87  | 10.35    | 9.248     |
| 72         | Hf      | 65.37  | 11.28  | 10.75    | 9.567     |
| 73         | Ta      | 67.46  | 11.68  | 11.14    | 9.883     |
| 74         | W       | 69.51  | 12.09  | 11.54    | 10.20     |
| 75         | Re      | 71.67  | 12.52  | 11.96    | 10.53     |
| 76         | Os      | 73.87  | 12.97  | 12.38    | 10.86     |
| 77         | Ir      | 76.11  | 13.41  | 12.82    | 11.21     |
| 78         | Pt      | 78.35  | 13.865 | 13.26    | 11.55     |
| 79         | Au      | 80.67  | 14.351 | 13.731   | 11.92     |
| 80         | Hg      | 83.08  | 14.838 | 14.205   | 12.278    |
| 81         | Tl      | 85.52  | 15.344 | 14.695   | 12.65     |
| 82         | Pb      | 87.95  | 15.861 | 15.200   | 13.03     |
| 83         | Bi      | 90.54  | 16.386 | 15.709   | 13.42     |
| 84         | Po      | 93.16  | 16.925 | 16.233   | 13.81     |
| 85         | At      | 95.73  | 17.481 | 16.777   | 14.21     |



**TABLE 7.3** Critical X-Ray Absorption Energies in keV (*Continued*)

| Atomic No. | Element | $K$   | $L_1$  | $L_{II}$ | $L_{III}$ |
|------------|---------|-------|--------|----------|-----------|
| 86         | Rn      | 98.45 | 18.054 | 17.331   | 14.61     |
| 87         | Fa      | 101.1 | 18.628 | 17.893   | 15.02     |
| 88         | Ra      | 103.9 | 19.228 | 18.473   | 15.44     |
| 89         | Ac      | 107.7 | 19.829 | 19.071   | 15.86     |
| 90         | Th      | 109.8 | 20.452 | 19.673   | 16.278    |
| 91         | Pa      | 112.4 | 21.096 | 20.295   | 16.720    |
| 92         | U       | 115.0 | 21.757 | 20.944   | 17.163    |
| 93         | Np      | 118.2 | 22.411 | 21.585   | 17.606    |
| 94         | Pu      | 121.2 | 23.117 | 22.250   | 18.062    |
| 95         | Am      | 124.3 | 23.795 | 22.935   | 18.524    |
| 96         | Cm      | 127.2 | 24.502 | 23.629   | 18.992    |
| 97         | Bk      | 131.3 | 25.231 | 24.344   | 19.466    |
| 98         | Cf      | 133.6 | 26.010 | 25.070   | 19.954    |
| 99         | Es      | 138.1 | 26.729 | 25.824   | 20.422    |
| 100        | Fm      | 141.5 | 27.503 | 26.584   | 20.912    |

**TABLE 7.4** X-Ray Emission Energies in keV

| Atomic No. | Element | $K\beta_1$ | $K\alpha_1$ | $L\beta_1$ | $L\alpha_1$ |
|------------|---------|------------|-------------|------------|-------------|
| 3          | Li      |            | 0.052       |            |             |
| 4          | Be      |            | 0.110       |            |             |
| 5          | B       |            | 0.185       |            |             |
| 6          | C       |            | 0.282       |            |             |
| 7          | N       |            | 0.392       |            |             |
| 8          | O       |            | 0.523       |            |             |
| 9          | F       |            | 0.677       |            |             |
| 10         | Ne      |            | 0.851       |            |             |
| 11         | Na      | 1.067      | 1.041       |            |             |
| 12         | Mg      | 1.297      | 1.254       |            |             |
| 13         | Al      | 1.553      | 1.487       |            |             |
| 14         | Si      | 1.832      | 1.740       |            |             |
| 15         | P       | 2.136      | 2.015       |            |             |
| 16         | S       | 2.464      | 2.308       |            |             |
| 17         | Cl      | 2.815      | 2.622       |            |             |
| 18         | Ar      | 3.192      | 2.957       |            |             |
| 19         | K       | 3.589      | 3.313       |            |             |
| 20         | Ca      | 4.012      | 3.691       | 0.344      | 0.341       |
| 21         | Sc      | 4.460      | 4.090       | 0.399      | 0.395       |
| 22         | Ti      | 4.931      | 4.510       | 0.458      | 0.452       |
| 23         | V       | 5.427      | 4.952       | 0.519      | 0.512       |

**TABLE 7.4** X-Ray Emission Energies in keV (*Continued*)

| Atomic No. | Element | $K\beta_1$ | $K\alpha_1$ | $L\beta_1$ | $L\alpha_1$ |
|------------|---------|------------|-------------|------------|-------------|
| 24         | Cr      | 5.946      | 5.414       | 0.581      | 0.571       |
| 25         | Mn      | 6.490      | 5.898       | 0.647      | 0.636       |
| 26         | Fe      | 7.057      | 6.403       | 0.717      | 0.704       |
| 27         | Co      | 7.649      | 6.930       | 0.790      | 0.775       |
| 28         | Ni      | 8.264      | 7.477       | 0.866      | 0.849       |
| 29         | Cu      | 8.904      | 8.047       | 0.948      | 0.928       |
| 30         | Zn      | 9.571      | 8.638       | 1.032      | 1.009       |
| 31         | Ga      | 10.263     | 9.251       | 1.122      | 1.096       |
| 32         | Ge      | 10.981     | 9.885       | 1.216      | 1.186       |
| 33         | As      | 11.725     | 10.543      | 1.317      | 1.282       |
| 34         | Se      | 12.495     | 11.221      | 1.419      | 1.379       |
| 35         | Br      | 13.290     | 11.923      | 1.526      | 1.480       |
| 36         | Kr      | 14.112     | 12.649      | 1.638      | 1.587       |
| 37         | Rb      | 14.960     | 13.394      | 1.752      | 1.694       |
| 38         | Sr      | 15.834     | 14.164      | 1.872      | 1.806       |
| 39         | Y       | 16.736     | 14.957      | 1.996      | 1.922       |
| 40         | Zr      | 17.666     | 15.774      | 2.124      | 2.042       |
| 41         | Nb      | 18.621     | 16.614      | 2.257      | 2.166       |
| 42         | Mo      | 19.607     | 17.478      | 2.395      | 2.293       |
| 43         | Tc      | 20.612     | 18.370      | 2.538      | 2.424       |
| 44         | Ru      | 21.655     | 19.278      | 2.683      | 2.558       |
| 45         | Rh      | 22.721     | 20.214      | 2.834      | 2.696       |
| 46         | Pd      | 23.816     | 21.175      | 2.990      | 2.838       |
| 47         | Ag      | 24.942     | 22.162      | 3.151      | 2.984       |
| 48         | Cd      | 26.093     | 23.172      | 3.316      | 3.133       |
| 49         | In      | 27.274     | 24.207      | 3.487      | 3.287       |
| 50         | Sn      | 28.483     | 25.270      | 3.662      | 3.444       |
| 51         | Sb      | 29.723     | 26.357      | 3.843      | 3.605       |
| 52         | Te      | 30.993     | 27.471      | 4.029      | 3.769       |
| 53         | I       | 32.292     | 28.610      | 4.220      | 3.937       |
| 54         | Xe      | 33.644     | 29.779      | 4.422      | 4.111       |
| 55         | Cs      | 34.984     | 30.970      | 4.620      | 4.286       |
| 56         | Ba      | 36.376     | 32.191      | 4.828      | 4.467       |
| 57         | La      | 37.799     | 33.440      | 5.043      | 4.651       |
| 58         | Ce      | 39.255     | 34.717      | 5.262      | 4.840       |
| 59         | Pr      | 40.746     | 36.023      | 5.489      | 5.034       |
| 60         | Nd      | 42.269     | 37.359      | 5.722      | 5.230       |
| 61         | Pm      | 43.811     | 38.726      | 5.956      | 5.431       |
| 62         | Sm      | 45.400     | 40.124      | 6.206      | 5.636       |
| 63         | Eu      | 47.027     | 41.529      | 6.456      | 5.846       |
| 64         | Gd      | 48.718     | 42.983      | 6.714      | 6.059       |
| 65         | Tb      | 50.391     | 44.470      | 6.979      | 6.275       |

**TABLE 7.4** X-Ray Emission Energies in keV (*Continued*)

| Atomic No. | Element | $K\beta_1$ | $K\alpha_1$ | $L\beta_1$ | $L\alpha_1$ |
|------------|---------|------------|-------------|------------|-------------|
| 66         | Dy      | 52.178     | 45.985      | 7.249      | 6.495       |
| 67         | Ho      | 53.934     | 47.528      | 7.528      | 6.720       |
| 68         | Er      | 55.690     | 49.099      | 7.810      | 6.948       |
| 69         | Tm      | 57.487     | 50.730      | 8.103      | 7.181       |
| 70         | Yb      | 59.352     | 52.360      | 8.401      | 7.414       |
| 71         | Lu      | 61.282     | 54.063      | 8.708      | 7.654       |
| 72         | Hf      | 63.209     | 55.757      | 9.021      | 7.898       |
| 73         | Ta      | 65.210     | 57.524      | 9.341      | 8.145       |
| 74         | W       | 67.233     | 59.310      | 9.670      | 8.396       |
| 75         | Re      | 69.298     | 61.131      | 10.008     | 8.651       |
| 76         | Os      | 71.404     | 62.991      | 10.354     | 8.910       |
| 77         | Ir      | 73.549     | 64.886      | 10.706     | 9.173       |
| 78         | Pt      | 75.736     | 66.820      | 11.069     | 9.441       |
| 79         | Au      | 77.968     | 68.794      | 11.439     | 9.711       |
| 80         | Hg      | 80.258     | 70.821      | 11.823     | 9.987       |
| 81         | Tl      | 82.558     | 72.860      | 12.210     | 10.266      |
| 82         | Pb      | 84.922     | 74.957      | 12.611     | 10.549      |
| 83         | Bi      | 87.335     | 77.097      | 13.021     | 10.836      |
| 84         | Po      | 89.809     | 79.296      | 13.441     | 11.128      |
| 85         | At      | 92.319     | 81.525      | 13.873     | 11.424      |
| 86         | Rn      | 94.877     | 83.800      | 14.316     | 11.724      |
| 87         | Fr      | 97.483     | 86.119      | 14.770     | 12.029      |
| 88         | Ra      | 100.136    | 88.485      | 15.233     | 12.338      |
| 89         | Ac      | 102.846    | 90.894      | 15.712     | 12.650      |
| 90         | Th      | 105.592    | 93.334      | 16.200     | 12.966      |
| 91         | Pa      | 108.408    | 95.851      | 16.700     | 13.291      |
| 92         | U       | 111.289    | 98.428      | 17.218     | 13.613      |
| 93         | Np      | 114.181    | 101.005     | 17.740     | 13.945      |
| 94         | Pu      | 117.146    | 103.653     | 18.278     | 14.279      |
| 95         | Am      | 120.163    | 106.351     | 18.829     | 14.618      |
| 96         | Cm      | 123.235    | 109.098     | 19.393     | 14.961      |
| 97         | Bk      | 126.362    | 111.896     | 19.971     | 15.309      |
| 98         | Cf      | 129.544    | 114.745     | 20.562     | 15.661      |
| 99         | Es      | 132.781    | 117.646     | 21.166     | 16.018      |
| 100        | Fm      | 136.075    | 120.598     | 21.785     | 16.379      |

of that of the corresponding  $K\alpha_1$  radiation. In practical applications these ratios have to be corrected for differential absorption in the window of the tube and air path, the ratio of scattering factors for and differential absorption in the crystal, and for sensitivity characteristics of the detector. Generalizing, the intensities of radiations from the  $K$  and  $L$  series are as follows:

| Emission line      | $K\alpha_1$ | $K\alpha_2$ | $K\beta_1$ | $K\beta_2$ | $L\alpha_1$ | $L\alpha_2$ | $L\beta_1$ | $L\beta_2$ | $L\gamma_1$ |
|--------------------|-------------|-------------|------------|------------|-------------|-------------|------------|------------|-------------|
| Relative intensity | 500         | 250         | 80–150     | 5          | 100         | 10          | 30         | 60         | 40          |

For angles at which the  $K\alpha_1$ ,  $K\alpha_2$  doublet is not resolved, a mean wavelength [ $K\bar{\alpha} = (2K\alpha_1 + K\alpha_2)/3$ ] can be used.

**Filters.** The  $K$  spectra of the light metals, often used as target material in the production of X-rays for diffraction studies, contain three strong lines,  $\alpha_1$ ,  $\alpha_2$  and  $\beta_1$ , of which the  $\alpha$  lines form a doublet with a narrow wavelength separation. The  $K\beta$  radiation can be eliminated by using a thin foil filter, usually of the element of next lower atomic number to that of the target element: the  $K\alpha$  lines are transmitted with a relatively small loss of intensity. Table 7.5, restricted to the  $K$  wavelengths of target elements in common use, lists the calculated thicknesses of  $\beta$  filters required to reduce the  $K\beta_1/K\alpha_1$  integrated intensity ratio to  $1/100$ .

**Interplanar Spacings.** Diffractometer alignment procedures require the use of a well-prepared polycrystalline specimen. Two standard samples found to be suitable are silicon and  $\alpha$ -quartz (including Novaculite). The  $2\theta$  values of several of the most intense reflections for these materials are listed in Table 7.6 (*Tables of Interplanar Spacings  $d$  vs. Diffraction Angle  $2\theta$  for Selected Targets*, Picker Nuclear, White Plains, N.Y., 1966). To convert to  $d$  for  $K\bar{\alpha}$  or to  $d$  for  $K\alpha_2$ , multiply the tabulated  $d$  value (Table 7.6) for  $K\alpha_1$  by the factor given below:

| Element | $K\bar{\alpha}$ | $K\alpha_2$ |
|---------|-----------------|-------------|
| W       | 1.007 69        | 1.023 07    |
| Ag      | 1.002 63        | 1.007 89    |
| Mo      | 1.002 02        | 1.006 04    |
| Cu      | 1.000 82        | 1.002 48    |
| Ni      | 1.000 77        | 1.002 32    |
| Co      | 1.000 72        | 1.002 16    |
| Fe      | 1.000 67        | 1.002 04    |
| Cr      | 1.000 57        | 1.001 70    |

**Analyzing Crystals.** The range of wavelengths usable with various analyzing crystals are governed by the  $d$  spacings of the crystal planes and by the geometric limits to which the goniometer can be rotated. The  $d$  value should be small enough to make the angle  $2\theta$  greater than approximately 10 or 15 deg, even at the shortest wavelength used: otherwise excessively long analyzing crystals would be needed to prevent the direct fluorescent beam from entering the detector. A small  $d$  value is also favorable for producing a large dispersion of the spectrum to give good separation of adjacent lines. On the other hand, a small  $d$  value imposes an upper limit to the range of wavelengths that can be analyzed. Actually the goniometer is limited mechanically to about 150 deg for a  $2\theta$  value. A final requirement is the reflection efficiency and minimization of higher-order reflections. Table 7.7 gives a list of crystals commonly used for X-ray spectroscopy.

TABLE 7.5  $\beta$  Filters for Common Target Elements

| Target<br>Element | $K\bar{\alpha}$ , Å | Excitation<br>Voltage, keV | $K\beta_1\ K\alpha_1 = 1/100$ |                  |                   | % Loss<br>$K\alpha_1$ |
|-------------------|---------------------|----------------------------|-------------------------------|------------------|-------------------|-----------------------|
|                   |                     |                            | Absorber                      | Thickness,<br>mm | g/cm <sup>2</sup> |                       |
| Ag                | 0.560834            | 25.52                      | Pd                            | 0.062            | 0.074             | 60                    |
| Mo                | 0.71069             | 20.00                      | Zr                            | 0.081            | 0.053             | 57                    |
| Cu                | 1.54178             | 8.981                      | Ni                            | 0.015            | 0.013             | 45                    |
| Ni                | 1.65912             | 8.331                      | Co                            | 0.013            | 0.011             | 42                    |
| Co                | 1.79021             | 7.709                      | Fe                            | 0.012            | 0.009             | 39                    |
| Fe                | 1.93728             | 7.111                      | Mn                            | 0.011            | 0.008             | 38                    |
| Cr                | 2.29092             | 5.989                      | MnO <sub>2</sub>              | 0.026            | 0.013             | 45                    |
|                   |                     |                            | V                             | 0.011            | 0.007             | 37                    |
|                   |                     |                            | V <sub>2</sub> O <sub>5</sub> | 0.036            | 0.012             | 48                    |
|                   | $L\alpha_1$         |                            | $L\beta_1\ L\alpha_1 = 1/100$ |                  |                   | % Loss<br>$L\alpha_1$ |
| W                 | 1.4763              | 10.200                     | Cu                            | 0.035            |                   | 77                    |

TABLE 7.6 Interplanar Spacings for  $K\alpha_1$  Radiation,  $d$  versus  $2\theta$

| $\alpha$ -quartz (Including Novaculite) |               |                |                |                 |                |               |                   |                 |                 |                 |
|-----------------------------------------|---------------|----------------|----------------|-----------------|----------------|---------------|-------------------|-----------------|-----------------|-----------------|
| $hkl$<br>$d(\text{\AA})$                | 100<br>4.260  | 101<br>3.343   | 110<br>2.458   | 102<br>2.282    | 200<br>2.128   | 112<br>1.817  | 202<br>1.672      | 211<br>1.541    | 203<br>1.375    | 301<br>1.372    |
| W $K\alpha_1: 2\theta$                  | 2.81          | 3.58           | 4.87           | 5.25            | 5.63           | 6.59          | 7.17              | 7.78            | 8.72            | 8.74            |
| Ag $K\alpha_1: 2\theta$                 | 7.53          | 9.60           | 13.07          | 14.08           | 15.10          | 17.71         | 19.26             | 20.91           | 23.47           | 23.52           |
| Mo $K\alpha_1: 2\theta$                 | 9.55          | 12.18          | 16.59          | 17.88           | 19.19          | 22.51         | 24.49             | 26.61           | 29.89           | 29.96           |
| Cu $K\alpha_1: 2\theta$                 | 20.83         | 26.64          | 36.52          | 39.45           | 42.44          | 50.16         | 54.86             | 59.98           | 68.14           | 68.31           |
| Ni $K\alpha_1: 2\theta$                 | 22.44         | 28.71          | 39.42          | 42.60           | 45.85          | 54.28         | 59.44             | 65.08           | 74.15           | 74.34           |
| Co $K\alpha_1: 2\theta$                 | 24.24         | 31.04          | 42.68          | 46.15           | 49.71          | 58.98         | 64.68             | 70.96           | 81.16           | 81.38           |
| Fe $K\alpha_1: 2\theta$                 | 26.27         | 33.66          | 46.38          | 50.20           | 54.11          | 64.38         | 70.75             | 77.83           | 89.50           | 89.74           |
| Cr $K\alpha_1: 2\theta$                 | 31.18         | 40.05          | 55.52          | 60.22           | 65.09          | 78.11         | 86.42             | 95.96           | 112.73          | 113.11          |
| Silicon                                 |               |                |                |                 |                |               |                   |                 |                 |                 |
| $hkl$<br>$d(\text{\AA})$                | 111<br>3.1353 | 220<br>1.91997 | 311<br>1.63736 | 400<br>1.357630 | 331<br>1.24584 | 422<br>1.1085 | 511,333<br>1.0451 | 440<br>0.959986 | 531<br>0.917922 | 620<br>0.858637 |
| W $K\alpha_1: 2\theta$                  | 3.82          | 6.24           | 7.32           | 8.83            | 9.62           | 10.82         | 11.48             | 12.50           | 13.07           | 13.98           |
| Ag $K\alpha_1: 2\theta$                 | 10.24         | 16.75          | 19.67          | 23.78           | 25.95          | 29.23         | 31.04             | 33.88           | 35.48           | 38.02           |
| Mo $K\alpha_1: 2\theta$                 | 12.99         | 21.29          | 25.02          | 30.28           | 33.08          | 37.32         | 39.67             | 43.36           | 45.45           | 48.79           |
| Cu $K\alpha_1: 2\theta$                 | 28.44         | 47.30          | 56.12          | 69.13           | 76.38          | 88.03         | 94.96             | 106.71          | 114.10          | 127.55          |
| Ni $K\alpha_1: 2\theta$                 | 30.66         | 51.16          | 60.83          | 75.26           | 83.42          | 96.80         | 104.96            | 119.42          | 129.12          | 149.76          |
| Co $K\alpha_1: 2\theta$                 | 33.15         | 55.53          | 66.22          | 82.42           | 91.77          | 107.59        | 117.71            | 137.42          | 154.04          |                 |
| Fe $K\alpha_1: 2\theta$                 | 35.97         | 60.55          | 72.48          | 90.96           | 101.97         | 121.67        | 135.70            |                 |                 |                 |
| Cr $K\alpha_1: 2\theta$                 | 42.83         | 73.21          | 88.72          | 114.97          | 133.53         |               |                   |                 |                 |                 |

**TABLE 7.7** Analyzing Crystals for X-Ray Spectroscopy

| Crystal                             | Reflecting Plane | $2d$ Spacing, Å | Reflectivity |
|-------------------------------------|------------------|-----------------|--------------|
| Quartz                              | 505 $\bar{2}$    | 1.624           | Low          |
| Aluminum                            | 111              | 2.338           | High         |
| Topaz                               | 303              | 2.712           | Medium       |
| Quartz                              | 20 $\bar{2}$ 3   | 2.750           | Low          |
| Lithium fluoride                    | 220              | 2.848           | High         |
| Silicon                             | 111              | 3.135           | High         |
| Quartz                              | 112              | 3.636           | Medium       |
| Lithium fluoride                    | 200              | 4.028           | High         |
| Sodium chloride                     | 200              | 5.639           | High         |
| Calcium fluoride                    | 111              | 6.32            | High         |
| Quartz                              | 10 $\bar{1}$ 1   | 6.686           | High         |
| Quartz                              | 10 $\bar{1}$ 0   | 8.50            | Medium       |
| Pentaerythritol (PET)               | 002              | 8.742           | High         |
| Ethylenediamine tartrate (EDT)      | 020              | 8.808           | Medium       |
| Ammonium dihydrogen phosphate (ADP) | 110              | 10.648          | Low          |
| Gypsum                              | 020              | 15.185          | Medium       |
| Mica                                | 002              | 19.92           | Low          |
| Potassium hydrogen phthalate (KAP)  | 10 $\bar{1}$ 1   | 26.4            | Medium       |
| Lead palmitate                      |                  | 45.6            |              |
| Strontium behenate                  |                  | 61.3            |              |
| Lead stearate                       |                  | 100.4           | Medium       |

The long-wavelength analyzers are prepared by dipping an optical flat into the film of the metal fatty acid about 50 times to produce a layer 180 molecules in thickness.

Lithium fluoride is the optimum crystal for all wavelengths less than 3 Å. Pentaerythritol (PET) and potassium hydrogen phthalate (KAP) are usually the crystals of choice for wavelengths from 3 to 20 Å. Two crystals suppress even-ordered reflections: silicon (111) and calcium fluoride (111).

**Mass Absorption Coefficients.** Radiation traversing a layer of substance is diminished in intensity by a constant fraction per centimeter thickness  $x$  of material. The emergent radiant power  $P$ , in terms of incident radiant power  $P_0$ , is given by

$$P = P_0 \exp(-\mu x)$$

which defines the total linear absorption coefficient  $\mu$ . Since the reduction of intensity is determined by the quantity of matter traversed by the primary beam, the absorber thickness is best expressed on a mass basis, in g/cm<sup>2</sup>. The mass absorption coefficient  $\mu/\rho$ , expressed in units cm<sup>2</sup>/g, where  $\rho$  is the density of the material, is approximately independent of the physical state of the material and, to a good approximation, is additive with respect to the elements composing a substance.

Table 7.8 contains values of  $\mu/\rho$  for the common target elements employed in X-ray work. A more extensive set of mass absorption coefficients for  $K$ ,  $L$ , and  $M$  emission lines within the wavelength range from 0.7 to 12 Å is contained in Heinrich's paper in T. D. McKinley, K. F. J. Heinrich, and D. B. Wittry (eds.), *The Electron Microprobe*, Wiley, New York, 1966, pp. 351–377. This article should be consulted to ascertain the probable accuracy of the values and for a compilation of coefficients and exponents employed in the computations.

TABLE 7.8 Mass Absorption Coefficients for  $K\alpha_1$  Lines and  $W L\alpha_1$  Line

| Emitter<br>wavelength, Å | Ag $K\alpha_1$<br>0.559 | Mo $K\alpha_1$<br>0.709 | Cu $K\alpha_1$<br>1.541 | Ni $K\alpha_1$<br>1.658 | Co $K\alpha_1$<br>1.789 | Fe $K\alpha_1$<br>1.936 | Cr $K\alpha_1$<br>2.290 | W $L\alpha_1$<br>1.476 |
|--------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|------------------------|
| Absorber                 |                         |                         |                         |                         |                         |                         |                         |                        |
| 1 H                      | 0.37                    | 0.38                    | 0.43                    | 0.4                     | 0.4                     | 0.5                     | 0.5                     | 0.4                    |
| 2 He                     | 0.16                    | 0.18                    | 0.37                    | 0.4                     | 0.4                     | 0.5                     | 0.7                     | 0.3                    |
| 3 Li                     | 0.18                    | 0.22                    | 0.50                    | 0.6                     | 0.7                     | 0.9                     | 1.5                     | 0.4                    |
| 4 Be                     | 0.22                    | 0.30                    | 1.2                     | 1.5                     | 1.9                     | 2.3                     | 3.7                     | 1.1                    |
| 5 B                      | 0.30                    | 0.45                    | 2.5                     | 3.1                     | 3.9                     | 4.9                     | 7.9                     | 2.2                    |
| 6 C                      | 0.42                    | 0.50                    | 4.6                     | 5.7                     | 7.1                     | 8.8                     | 14.2                    | 4.1                    |
| 7 N                      | 0.60                    | 0.83                    | 7.5                     | 9.3                     | 11.5                    | 14.4                    | 23.1                    | 6.7                    |
| 8 O                      | 0.80                    | 1.45                    | 12.9                    | 15.8                    | 19.5                    | 24.5                    | 39.4                    | 11.4                   |
| 9 F                      | 1.00                    | 1.9                     | 16.5                    | 20.3                    | 25.2                    | 31.4                    | 50.3                    | 14.6                   |
| 10 Ne                    | 1.41                    | 2.6                     | 22.8                    | 27.9                    | 34.6                    | 43.1                    | 69.0                    | 20.1                   |
| 11 Na                    | 1.75                    | 3.5                     | 30.3                    | 37.2                    | 45.9                    | 57.2                    | 91.4                    | 26.8                   |
| 12 Mg                    | 2.27                    | 4.6                     | 39.5                    | 48.4                    | 59.8                    | 74.6                    | 119.1                   | 34.9                   |
| 13 Al                    | 2.74                    | 5.8                     | 49.6                    | 60.7                    | 75.0                    | 93.4                    | 149.0                   | 43.9                   |
| 14 Si                    | 3.44                    | 7.3                     | 61.4                    | 75.2                    | 92.8                    | 115.5                   | 183.8                   | 54.4                   |
| 15 P                     | 4.20                    | 8.8                     | 74.7                    | 91.4                    | 112.9                   | 140.5                   | 223.6                   | 66.2                   |
| 16 S                     | 5.15                    | 10.6                    | 89.2                    | 109.2                   | 134.7                   | 167.4                   | 266.1                   | 79.1                   |
| 17 Cl                    | 5.86                    | 12.4                    | 104.8                   | 128.2                   | 158.1                   | 196.6                   | 312.4                   | 92.8                   |
| 18 Ar                    | 6.40                    | 14.5                    | 121.4                   | 148.5                   | 183.0                   | 227.3                   | 360.7                   | 107.6                  |
| 19 K                     | 8.0                     | 16.7                    | 139.8                   | 171                     | 211                     | 262                     | 415                     | 124                    |
| 20 Ca                    | 9.7                     | 18.9                    | 158.6                   | 194                     | 239                     | 296                     | 469                     | 141                    |
| 21 Sc                    | 10.5                    | 21.8                    | 180.5                   | 221                     | 272                     | 337                     | 534                     | 160                    |
| 22 Ti                    | 11.8                    | 25.3                    | 203                     | 247                     | 304                     | 378                     | 597                     | 180                    |
| 23 V                     | 13.3                    | 27.7                    | 228                     | 278                     | 342                     | 424                     | 77                      | 202                    |
| 24 Cr                    | 15.7                    | 31.0                    | 254                     | 311                     | 382                     | 474                     | 88                      | 226                    |
| 25 Mn                    | 17.4                    | 34.5                    | 282                     | 344                     | 423                     | 63.5                    | 101                     | 250                    |
| 26 Fe                    | 19.9                    | 38.1                    | 311                     | 380                     | 57.6                    | 71.4                    | 113                     | 276                    |
| 27 Co                    | 21.8                    | 42.1                    | $K$ 341                 | 52.8                    | 64.9                    | 80.6                    | 127                     | 303                    |
| 28 Ni                    | 25.0                    | 46.4                    | 48.3                    | 58.9                    | 72.5                    | 90.0                    | 142                     | 333                    |
| 29 Cu                    | 26.4                    | 50.7                    | 53.7                    | 65.5                    | 80.6                    | 100.0                   | 158                     | 47.6                   |
| 30 Zn                    | 28.2                    | 55.4                    | 59.5                    | 72.7                    | 89.4                    | 110.9                   | 175                     | 52.8                   |
| 31 Ga                    | 30.8                    | 60.1                    | 65.9                    | 80.5                    | 99.0                    | 122.8                   | 194                     | 58.5                   |
| 32 Ge                    | 33.5                    | 65.2                    | 72.3                    | 88.2                    | 108.6                   | 134.7                   | 213                     | 64.1                   |
| 33 As                    | 36.5                    | 70.5                    | 79.1                    | 96.6                    | 118.9                   | 147                     | 233                     | 70.2                   |
| 34 Se                    | 38.5                    | 76.0                    | 86.1                    | 105.1                   | 129.4                   | 161                     | 254                     | 76.4                   |
| 35 Br                    | 42.3                    | 82.5                    | 93.9                    | 114.7                   | 141.2                   | 175                     | 277                     | 83.4                   |
| 36 Kr                    | 45.0                    | 88.3                    | 101.9                   | 124.5                   | 153.2                   | 190                     | 300                     | 90.5                   |
| 37 Rb                    | 48                      | 95                      | 84                      | 103                     | 127                     | 158                     | 252                     | 98                     |
| 38 Sr                    | 52                      | 102                     | 90                      | 110                     | 137                     | 170                     | 271                     | 106                    |

**TABLE 7.8** Mass Absorption Coefficients for  $K\alpha_1$  Lines and W  $L\alpha_1$  Line (*Continued*)

| Emitter<br>wavelength, Å | Ag $K\alpha_1$<br>0.559 | Mo $K\alpha_1$<br>0.709 | Cu $K\alpha_1$<br>1.541 | Ni $K\alpha_1$<br>1.658 | Co $K\alpha_1$<br>1.789 | Fe $K\alpha_1$<br>1.936 | Cr $K\alpha_1$<br>2.290 | W $L\alpha_1$<br>1.476 |
|--------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|------------------------|
| Absorber                 |                         |                         |                         |                         |                         |                         |                         |                        |
| 39 Y                     | 56                      | 109                     | 97                      | 119                     | 147                     | 183                     | 292                     | 114                    |
| 40 Zr                    | 61                      | 17                      | 104                     | 128                     | 158                     | 197                     | 314                     | 122                    |
| 41 Nb                    | 66                      | 18                      | 112                     | 138                     | 170                     | 212                     | 338                     | 132                    |
| 42 Mo                    | 71                      | 19                      | 119                     | 146                     | 180                     | 225                     | 358                     | 140                    |
| 43 Tc                    | 76                      | 20                      | 128                     | 157                     | 194                     | 241                     | 384                     | 150                    |
| 44 Ru                    | 12                      | 22                      | 137                     | 168                     | 207                     | 258                     | 410                     | 160                    |
| 45 Rh                    | 13                      | 23                      | 146                     | 179                     | 221                     | 275                     | 438                     | 171                    |
| 46 Pd                    | 14                      | 24                      | 155                     | 190                     | 235                     | 292                     | 466                     | 182                    |
| 47 Ag                    | 15                      | 26                      | 165                     | 202                     | 249                     | 310                     | 493                     | 193                    |
| 48 Cd                    | 15                      | 28                      | 174                     | 213                     | 263                     | 327                     | 520                     | 204                    |
| 49 In                    | 16                      | 30                      | 185                     | 227                     | 280                     | 347                     | 553                     | 217                    |
| 50 Sn                    | 17                      | 32                      | 195                     | 239                     | 295                     | 367                     | 583                     | 229                    |
| 51 Sb                    | 19                      | 34                      | 206                     | 252                     | 310                     | 386                     | 612                     | 241                    |
| 52 Te                    | 19                      | 36                      | 216                     | 265                     | 326                     | 405                     | 644                     | 253                    |
| 53 I                     | 21                      | 37                      | 230                     | 281                     | 346                     | 431                     | 684                     | 269                    |
| 54 Xe                    | 22                      | 39                      | 239                     | 293                     | 361                     | 448                     | 710                     | 280                    |
| 55 Cs                    | 24                      | 42                      | 332                     | 404                     | 495                     | 612                     | 822                     | 295                    |
| 56 Ba                    | 25                      | 44                      | 349                     | 425                     | 522                     | 645                     | 622                     | 311                    |
| 57 La                    | 26                      | 46                      | 365                     | 444                     | 545                     | 673                     | 647                     | 325                    |
| 58 Ce                    | 28                      | 48                      | 383                     | 466                     | 571                     | 603                     | 216                     | 341                    |
| 59 Pr                    | 29                      | 51                      | 401                     | 487                     | 597                     | 453                     | 229                     | 356                    |
| 60 Nd                    | 31                      | 54                      | 420                     | 510                     | 534                     | 473                     | 241                     | 373                    |
| 61 Pm                    | 32                      | 56                      | 440                     | 535                     |                         | 164                     | 254                     | 392                    |
| 62 Sm                    | 33                      | 59                      | 456                     | 473                     | 417                     | 173                     | 268                     | 406                    |
| 63 Eu                    | 35                      | 61                      | 405                     | 354                     | 148                     | 182                     | 282                     | 423                    |
| 64 Gd                    | 36                      | 64                      | 424                     | 370                     | 156                     | 191                     | 296                     |                        |
| 65 Tb                    | 38                      | 67                      | 316                     | 135                     | 164                     | 201                     | 311                     | $393 L_I$              |
| 66 Dy                    | 39                      | 70                      | 329                     | 141                     | 172                     | 211                     | 327                     | $293 L_{II}$           |
| 67 Ho                    | 41                      | 72                      | 123                     | 148                     | 181                     | 222                     | 343                     | 304                    |
| 68 Er                    | 43                      | 75                      | 129                     | 156                     | 189                     | 233                     | 360                     | $316 L_{III}$          |
| 69 Tm                    | 45                      | 79                      | 135                     | 163                     | 199                     | 244                     | 377                     | 120                    |
| 70 Yb                    | 46                      | 82                      | 141                     | 171                     | 208                     | 256                     | 395                     | 126                    |
| 71 Lu                    | 48                      | 84                      | 148                     | 179                     | 218                     | 267                     | 414                     | 132                    |
| 72 Hf                    | 51                      | 88                      | 155                     | 187                     | 228                     | 280                     | 433                     | 138                    |
| 73 Ta                    | 52                      | 91                      | 162                     | 196                     | 238                     | 293                     | 453                     | 144                    |
| 74 W                     | 55                      | 95                      | 169                     | 204                     | 249                     | 306                     | 473                     | 151                    |
| 75 Re                    | 57                      | 98                      | 176                     | 213                     | 260                     | 319                     | 494                     | 157                    |
| 76 Os                    | 59                      | 102                     | 184                     | 223                     | 271                     | 333                     | 515                     | 164                    |
| 77 Ir                    | 61                      | 106                     | 192                     | 232                     | 283                     | 347                     | 538                     | 171                    |
| 78 Pt                    | 64                      | 109                     | 200                     | 242                     | 295                     | 362                     | 560                     | 179                    |



**TABLE 7.8** Mass Absorption Coefficients for  $K\alpha_1$  Lines and  $W L\alpha_1$  Line (*Continued*)

| Emitter wavelength, Å | Ag $K\alpha_1$<br>0.559 | Mo $K\alpha_1$<br>0.709 | Cu $K\alpha_1$<br>1.541 | Ni $K\alpha_1$<br>1.658 | Co $K\alpha_1$<br>1.789 | Fe $K\alpha_1$<br>1.936 | Cr $K\alpha_1$<br>2.290 | W $L\alpha_1$<br>1.476 |
|-----------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|------------------------|
| Absorber              |                         |                         |                         |                         |                         |                         |                         |                        |
| 79 Au                 | 67                      | 113                     | 209                     | 252                     | 307                     | 377                     | 584                     | 186                    |
| 80 Hg                 | 69                      | 117                     | 218                     | 263                     | 321                     | 394                     | 609                     | 194                    |
| 81 Tl                 | 72                      | 121                     | 227                     | 275                     | 334                     | 411                     | 635                     | 203                    |
| 82 Pb                 | 74                      | 125                     | 236                     | 286                     | 348                     | 428                     | 662                     | 211                    |
| 83 Bi                 | 78                      | 129                     | 247                     | 298                     | 363                     | 446                     | 690                     | 220                    |
| 84 Po                 |                         | 131                     | 258                     | 311                     | 380                     | 466                     | 721                     | 230                    |
| 85 At                 |                         |                         | 269                     | 325                     | 397                     | 487                     | 753                     | 240                    |
| 86 Rn                 | 85                      |                         | 281                     | 340                     | 414                     | 509                     | 787                     | 251                    |
| 87 Fr                 |                         | 89                      | 294                     | 356                     | 433                     | 532                     | 823                     | 262                    |
| 88 Ra                 | 91                      |                         | 307                     | 372                     | 453                     | 556                     | 861                     | 274                    |
| 89 Ac                 |                         |                         | 322                     | 389                     | 474                     | 582                     | 900                     | 287                    |
| 90 Th                 | 97                      |                         | 337                     | 408                     | 497                     | 610                     | 944                     | 301                    |
| 91 Pa                 |                         |                         | 353                     | 427                     | 520                     | 639                     | 988                     | 315                    |
| 92 U                  | 104                     |                         | 372                     | 450                     | 548                     | 673                     | 898                     | 332                    |
| 93 Np                 |                         |                         | 392                     | 474                     | 578                     | 709                     | 945                     | 350                    |
| 94 Pu                 |                         | 54                      | 418                     | 505                     | 615                     | 755                     | 835                     | 373                    |

## 7.2 ULTRAVIOLET-VISIBLE SPECTROSCOPY

Molecules with two or more isolated chromophores (absorbing groups) absorb light of nearly the same wavelength as does a molecule containing only a single chromophore of a particular type. The intensity of the absorption is proportional to the number of that type of chromophore present in the molecule. Representative chromophores are given in Table 7.9.

The solvent chosen must dissolve the sample, yet be relatively transparent in the spectral region of interest. In order to avoid poor resolution and difficulties in spectrum interpretation, a solvent should not be employed for measurements that are near the wavelength of or are shorter than the wavelength of its ultraviolet cutoff, that is, the wavelength at which absorbance for the solvent alone approaches one absorbance unit. Ultraviolet cutoffs for solvents commonly used are given in Table 7.10.

Appreciable interaction between chromophores does not occur unless they are linked directly to each other, or forced into close proximity as a result of molecular stereochemical configuration. Interposition of a single methylene group, or *meta* orientation about an aromatic ring, is sufficient to insulate chromophores almost completely from each other. Certain combinations of functional groups afford chromophoric systems which give rise to characteristic absorption bands.

Sets of empirical rules, often referred to as Woodward's rules or the Woodward-Fieser rules, enable the absorption maxima of dienes (Table 7.11) and enones and dienones (Table 7.12) to be predicted. To the respective base values (absorption wavelength of parent compound) are added the increments for the structural features or substituent groups present. When necessary, a solvent correction is also applied (Table 7.13).

**TABLE 7.9** Electronic Absorption Bands for Representative Chromophores

| Chromophore  | System                                     | $\lambda_{\max}$ | $\epsilon_{\max}$ |
|--------------|--------------------------------------------|------------------|-------------------|
| Acetylide    | $-\text{C}\equiv\text{C}-$                 | 175–180          | 6 000             |
| Aldehyde     | $-\text{CHO}$                              | 210              | strong            |
|              |                                            | 280–300          | 11–18             |
| Amine        | $-\text{NH}_2$                             | 195              | 2 800             |
| Azido        | $>\text{C}=\text{N}-$                      | 190              | 5 000             |
| Azo          | $-\text{N}=\text{N}-$                      | 285–400          | 3–25              |
| Bromide      | $-\text{Br}$                               | 208              | 300               |
| Carbonyl     | $>\text{C}=\text{O}$                       | 195              | 1 000             |
|              |                                            | 270–285          | 18–30             |
| Carboxyl     | $-\text{COOH}$                             | 200–210          | 50–70             |
| Disulfide    | $-\text{S}-\text{S}-$                      | 194              | 5 500             |
|              |                                            | 255              | 400               |
| Ester        | $-\text{COOR}$                             | 205              | 50                |
| Ether        | $-\text{O}-$                               | 185              | 1 000             |
| Ethylene     | $-\text{C}=\text{C}-$                      | 190              | 8 000             |
| Iodide       | $-\text{I}$                                | 260              | 400               |
| Nitrate      | $-\text{ONO}_2$                            | 270 (shoulder)   | 12                |
| Nitrile      | $-\text{C}\equiv\text{N}$                  | 160              | —                 |
| Nitrite      | $-\text{ONO}$                              | 220–230          | 1 000–2 000       |
|              |                                            | 300–400          | 10                |
| Nitro        | $-\text{NO}_2$                             | 210              | strong            |
| Nitroso      | $-\text{NO}$                               | 302              | 100               |
| Oxime        | $-\text{NOH}$                              | 190              | 5 000             |
| Sulfone      | $-\text{SO}_2-$                            | 180              | —                 |
| Sulfoxide    | $>\text{S}=\text{O}$                       | 210              | 1 500             |
| Thiocarbonyl | $>\text{C}=\text{S}$                       | 205              | strong            |
| Thioether    | $-\text{S}-$                               | 194              | 4 600             |
|              |                                            | 215              | 1 600             |
| Thiol        | $-\text{SH}$                               | 195              | 1 400             |
|              | $-(\text{C}=\text{C})_2-$ (acyclic)        | 210–230          | 21 000            |
|              | $-(\text{C}=\text{C})_3-$                  | 260              | 35 000            |
|              | $-(\text{C}=\text{C})_4-$                  | 300              | 52 000            |
|              | $-(\text{C}=\text{C})_5-$                  | 330              | 118 000           |
|              | $-(\text{C}=\text{C})_2-$ (alicyclic)      | 230–260          | 3 000–8 000       |
|              | $\text{C}=\text{C}-\text{C}\equiv\text{C}$ | 219              | 6 500             |
|              | $\text{C}=\text{C}-\text{C}=\text{N}$      | 220              | 23 000            |
|              | $\text{C}=\text{C}-\text{C}=\text{O}$      | 210–250          | 10 000–20 000     |
|              |                                            | 300–350          | weak              |
|              | $\text{C}=\text{C}-\text{NO}_2$            | 229              | 9 500             |
| Benzene      |                                            | 184              | 46 700            |
|              |                                            | 204              | 6 900             |
|              |                                            | 255              | 170               |
| Diphenyl     |                                            | 246              | 20 000            |
| Naphthalene  |                                            | 222              | 112 000           |
|              |                                            | 275              | 5 600             |
|              |                                            | 312              | 175               |
| Anthracene   |                                            | 252              | 199 000           |
|              |                                            | 375              | 7 900             |
| Phenanthrene |                                            | 251              | 66 000            |
|              |                                            | 292              | 14 000            |
| Naphthacene  |                                            | 272              | 180 000           |
|              |                                            | 473              | 12 500            |

**TABLE 7.9** Electronic Absorption Bands for Representative Chromophores (*Continued*)

| Chromophore  | System | $\lambda_{\text{max}}$ | $\epsilon_{\text{max}}$ |
|--------------|--------|------------------------|-------------------------|
| Pentacene    |        | 310                    | 300 000                 |
|              |        | 585                    | 12 000                  |
| Pyridine     |        | 174                    | 80 000                  |
|              |        | 195                    | 6 000                   |
| Quinoline    |        | 257                    | 1 700                   |
|              |        | 227                    | 37 000                  |
|              |        | 270                    | 3 600                   |
|              |        | 314                    | 2 750                   |
| Isoquinoline |        | 218                    | 80 000                  |
|              |        | 266                    | 4 000                   |
|              |        | 317                    | 3 500                   |

**TABLE 7.10** Ultraviolet Cutoffs of Spectrograde Solvents

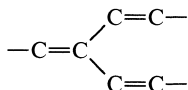
*Absorbance of 1.00 in a 10.0 mm cell vs. distilled water.*

| Solvent                                 | Wavelength,<br>nm | Solvent                                         | Wavelength,<br>nm |
|-----------------------------------------|-------------------|-------------------------------------------------|-------------------|
| Acetic acid                             | 260               | Hexadecane                                      | 200               |
| Acetone                                 | 330               | Hexane                                          | 210               |
| Acetonitrile                            | 190               | Isobutyl alcohol                                | 230               |
| Benzene                                 | 280               | Methanol                                        | 210               |
| 1-Butanol                               | 210               | 2-Methoxyethanol                                | 210               |
| 2-Butanol                               | 260               | Methylcyclohexane                               | 210               |
| Butyl acetate                           | 254               | Methylene chloride                              | 235               |
| Carbon disulfide                        | 380               | Methyl ethyl ketone                             | 330               |
| Carbon tetrachloride                    | 265               | Methyl isobutyl ketone                          | 335               |
| 1-Chlorobutane                          | 220               | 2-Methyl-1-propanol                             | 230               |
| Chloroform (stabilized<br>with ethanol) | 245               | <i>N</i> -Methylpyrrolidone                     | 285               |
| Cyclohexane                             | 210               | Nitromethane                                    | 380               |
| 1,2-Dichloroethane                      | 226               | Pentane                                         | 210               |
| Diethyl ether                           | 218               | Pentyl acetate                                  | 212               |
| 1,2-Dimethoxyethane                     | 240               | 1-Propanol                                      | 210               |
| <i>N,N</i> -Dimethylacetamide           | 268               | 2-Propanol                                      | 210               |
| <i>N,N</i> -Dimethylformamide           | 270               | Pyridine                                        | 330               |
| Dimethylsulfoxide                       | 265               | Tetrachloroethylene<br>(stabilized with thymol) | 290               |
| 1,4-Dioxane                             | 215               | Tetrahydrofuran                                 | 220               |
| Ethanol                                 | 210               | Toluene                                         | 286               |
| 2-Ethoxyethanol                         | 210               | 1,1,2-Trichloro-1,2,2-<br>trifluoroethane       | 231               |
| Ethyl acetate                           | 255               | 2,2,4-Trimethylpentane                          | 215               |
| Ethylene chloride                       | 228               | <i>o</i> -Xylene                                | 290               |
| Glycerol                                | 207               | Water                                           | 191               |
| Heptane                                 | 197               |                                                 |                   |

**TABLE 7.11** Absorption Wavelength of Dienes

Heteroannular and acyclic dienes usually display molar absorptivities in the 8000 to 20 000 range, whereas homoannular dienes are in the 5000 to 8000 range.

Poor correlations are obtained for cross-conjugated polyene systems such as



The correlations presented here are sometimes referred to as Woodward's rules or the Woodward-Fieser rules.

|                                                      |       |
|------------------------------------------------------|-------|
| Base value for heteroannular or open chain diene, nm | 214   |
| Base value for homoannular diene, nm                 | 253   |
| Increment (in nm) for                                |       |
| double bond extending conjugation                    | 30    |
| Alkyl substituent or ring residue                    | 5     |
| Exocyclic double bond                                | 5     |
| Polar groupings:                                     |       |
| -O-acyl                                              | 0     |
| -O-alkyl                                             | 6     |
| -S-alkyl                                             | 30    |
| -Cl, -Br                                             | 5     |
| -N (alkyl) <sub>2</sub>                              | 60    |
| Solvent correction (see Table 7.13)                  | —     |
| Calculated wavelength =                              | total |

Ring substitution on the benzene ring affords shifts to longer wavelengths (Table 7.14) and intensification of the spectrum. With electron-withdrawing substituents, practically no change in the maximum position is observed. The spectra of heteroaromatics are related to their isocyclic analogs, but only in the crudest way. As with benzene, the magnitude of substituent shifts can be estimated, but tautomeric possibilities may invalidate the empirical method.

When electronically complementary groups are situated *para* to each other in disubstituted benzenes, there is a more pronounced shift to a longer wavelength than would be expected from the additive effect due to the extension of the chromophore from the electron-donating group through the ring to the electron-withdrawing group. When the *para* groups are not complementary, or when the groups are situated *ortho* or *meta* to each other, disubstituted benzenes show a more or less additive effect of the two substituents on the wavelength maximum. Calculation of the principal band of selected substituted benzenes is illustrated in Table 7.15.

**TABLE 7.12** Absorption Wavelength of Enones and Dienones

|                                                                                                 |  |  |                                                                                                                                                              |  |  |
|-------------------------------------------------------------------------------------------------|--|--|--------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| $\text{O}=\text{C}-\overset{\alpha}{\underset{\beta}{\text{C}}}=\text{C}$                       |  |  | $\text{O}=\text{C}-\overset{\alpha}{\underset{\beta}{\text{C}}}=\overset{\gamma}{\underset{\delta}{\text{C}}}=\overset{\delta}{\underset{\delta}{\text{C}}}$ |  |  |
| Base values, nm                                                                                 |  |  |                                                                                                                                                              |  |  |
| Acyclic $\alpha,\beta$ -unsaturated ketones                                                     |  |  | 215                                                                                                                                                          |  |  |
| Acyclic $\alpha,\beta$ -unsaturated aldehyde                                                    |  |  | 210                                                                                                                                                          |  |  |
| Six-membered cyclic $\alpha,\beta$ -unsaturated ketones                                         |  |  | 215                                                                                                                                                          |  |  |
| Five-membered cyclic $\alpha,\beta$ -unsaturated ketones                                        |  |  | 214                                                                                                                                                          |  |  |
| $\alpha,\beta$ -Unsaturated carboxylic acids and esters                                         |  |  | 195                                                                                                                                                          |  |  |
| Increments (in nm) for                                                                          |  |  |                                                                                                                                                              |  |  |
| Double bond extending conjugation:                                                              |  |  |                                                                                                                                                              |  |  |
| Heteroannular                                                                                   |  |  | 30                                                                                                                                                           |  |  |
| Homoannular                                                                                     |  |  | 69                                                                                                                                                           |  |  |
| Alkyl group or ring residue:                                                                    |  |  |                                                                                                                                                              |  |  |
| $\alpha$                                                                                        |  |  | 10                                                                                                                                                           |  |  |
| $\beta$                                                                                         |  |  | 12                                                                                                                                                           |  |  |
| $\gamma, \delta$                                                                                |  |  | 18                                                                                                                                                           |  |  |
| Polar groups:                                                                                   |  |  |                                                                                                                                                              |  |  |
| —OH                                                                                             |  |  |                                                                                                                                                              |  |  |
| $\alpha$                                                                                        |  |  | 35                                                                                                                                                           |  |  |
| $\beta$                                                                                         |  |  | 30                                                                                                                                                           |  |  |
| $\gamma$                                                                                        |  |  | 50                                                                                                                                                           |  |  |
| —O—CO—CH <sub>3</sub> and —O—CO—C <sub>6</sub> H <sub>5</sub> : $\alpha, \beta, \gamma, \delta$ |  |  | 6                                                                                                                                                            |  |  |
| —OCH <sub>3</sub>                                                                               |  |  |                                                                                                                                                              |  |  |
| $\alpha$                                                                                        |  |  | 35                                                                                                                                                           |  |  |
| $\beta$                                                                                         |  |  | 30                                                                                                                                                           |  |  |
| $\gamma$                                                                                        |  |  | 17                                                                                                                                                           |  |  |
| $\delta$                                                                                        |  |  | 31                                                                                                                                                           |  |  |
| —S—alkyl, $\beta$                                                                               |  |  | 85                                                                                                                                                           |  |  |
| —Cl                                                                                             |  |  |                                                                                                                                                              |  |  |
| $\alpha$                                                                                        |  |  | 15                                                                                                                                                           |  |  |
| $\beta$                                                                                         |  |  | 12                                                                                                                                                           |  |  |
| —Br                                                                                             |  |  |                                                                                                                                                              |  |  |
| $\alpha$                                                                                        |  |  | 25                                                                                                                                                           |  |  |
| $\beta$                                                                                         |  |  | 30                                                                                                                                                           |  |  |
| —N(alkyl) <sub>2</sub> , $\beta$                                                                |  |  | 95                                                                                                                                                           |  |  |
| Exocyclic double bond                                                                           |  |  | 5                                                                                                                                                            |  |  |
| Solvent correction (see Table 7.13)                                                             |  |  |                                                                                                                                                              |  |  |
| Calculated wavelength =                                                                         |  |  | total                                                                                                                                                        |  |  |

**TABLE 7.13** Solvent Correction for Ultraviolet-Visible Spectroscopy

| Solvent       | Correction, nm |
|---------------|----------------|
| Chloroform    | + 1            |
| Cyclohexane   |                |
| Diethyl ether | + 11           |
| 1,4-Dioxane   | + 5            |
| Ethanol       | 0              |
| Hexane        | + 11           |
| Methanol      | 0              |
| Water         | − 8            |

**TABLE 7.14** Primary Bands of Substituted Benzene and Heteroaromatics*In methanol.*

Base value: 203.5 nm.

| Substituent                       | Wavelength shift, nm | Substituent                          | Wavelength shift, nm |
|-----------------------------------|----------------------|--------------------------------------|----------------------|
| —CH <sub>3</sub>                  | 3.0                  | —COOH                                | 25.5                 |
| —CH=CH <sub>2</sub>               | 44.5                 | —COO <sup>−</sup>                    | 20.5                 |
| —C≡CH                             | 44                   | —CN                                  | 20.5                 |
| —C <sub>6</sub> H <sub>5</sub>    | 48                   | —NH <sub>2</sub>                     | 26.5                 |
| —F                                | 0                    | —NH <sub>3</sub> <sup>+</sup>        | − 0.5                |
| —Cl                               | 6.0                  | —N(CH <sub>3</sub> ) <sub>2</sub>    | 47.0                 |
| —Br                               | 6.5                  | —NH—CO—CH <sub>3</sub>               | 38.5                 |
| —I                                | 3.5                  | —NO <sub>2</sub>                     | 57                   |
| —OH                               | 7.0                  | —SH                                  | 32                   |
| —O <sup>−</sup>                   | 31.5                 | —SO—C <sub>6</sub> H <sub>5</sub>    | 28                   |
| —OCH <sub>3</sub>                 | 13.5                 | —SO <sub>2</sub> CH <sub>3</sub>     | 13                   |
| —OC <sub>6</sub> H <sub>5</sub>   | 51.5                 | —SO <sub>2</sub> NH <sub>2</sub>     | 14.0                 |
| —CHO                              | 46.0                 | —CH=CH—C <sub>6</sub> H <sub>5</sub> |                      |
| —CO—CH <sub>3</sub>               | 42.0                 | <i>cis</i>                           | 79                   |
| —CO—C <sub>6</sub> H <sub>5</sub> | 48                   | <i>trans</i>                         | 92.0                 |
|                                   |                      | —CH=CH—COOH, <i>trans</i>            | 69.5                 |
| Heteroaromatic                    | Base value, nm       | Heteroaromatic                       | Base value, nm       |
| Furan                             | 200                  | Pyridine                             | 257                  |
| Pyrazine                          | 257                  | Pyrimidine                           | ca 235               |
| Pyrazole                          | 214                  | Pyrrole                              | 209                  |
| Pyridazine                        | ca 240               | Thiophene                            | 231                  |

**TABLE 7.15** Wavelength Calculation of the Principal Band of Substituted Benzene Derivatives*In ethanol.*


---

|                                                                             |     |
|-----------------------------------------------------------------------------|-----|
| Base value of parent chromophore, nm                                        |     |
| $\text{C}_6\text{H}_5\text{COOH}$ or $\text{C}_6\text{H}_5\text{COO—alkyl}$ | 230 |
| $\text{C}_6\text{H}_5\text{—CO—alkyl (or aryl)}$                            | 246 |
| $\text{C}_6\text{H}_5\text{CHO}$                                            | 250 |
| Increment (in nm) for each substituent on phenyl ring                       |     |
| —Alkyl or ring residue                                                      |     |
| <i>o-</i> , <i>m-</i>                                                       | 3   |
| <i>p-</i>                                                                   | 10  |
| —OH and —O— alkyl                                                           |     |
| <i>o-</i> , <i>m-</i>                                                       | 7   |
| <i>p-</i>                                                                   | 25  |
| —O—                                                                         |     |
| <i>o-</i>                                                                   | 11  |
| <i>m-</i>                                                                   | 20  |
| <i>p-</i>                                                                   | 78* |
| —Cl                                                                         |     |
| <i>o-</i> , <i>m-</i>                                                       | 0   |
| <i>p-</i>                                                                   | 10  |
| —Br                                                                         |     |
| <i>o-</i> , <i>m-</i>                                                       | 2   |
| <i>p-</i>                                                                   | 15  |
| —NH <sub>2</sub>                                                            |     |
| <i>o-</i> , <i>m-</i>                                                       | 13  |
| <i>p-</i>                                                                   | 58  |
| —NHCO—CH <sub>3</sub>                                                       |     |
| <i>o-</i> , <i>m-</i>                                                       | 20  |
| <i>p-</i>                                                                   | 45  |
| —NHCH <sub>3</sub>                                                          |     |
| <i>p-</i>                                                                   | 73  |
| —N(CH <sub>3</sub> ) <sub>2</sub>                                           |     |
| <i>o-</i> , <i>m-</i>                                                       | 20  |
| <i>p-</i>                                                                   | 85  |

---

\* Value may be decreased markedly by steric hindrance to coplanarity.

## 7.3 FLUORESCENCE

TABLE 7.16 Fluorescence Spectroscopy of Some Organic Compounds

| Compound                                | Solvent                            | pH   | Excitation wavelength, nm | Emission wavelength, nm |
|-----------------------------------------|------------------------------------|------|---------------------------|-------------------------|
| Acenaphthene                            | Pentane                            |      | 291                       | 341                     |
| Acridine                                | CF <sub>3</sub> COOH               |      | 358                       | 475                     |
| Adenine                                 | Water                              | 1    | 280                       | 375                     |
| Adenosine                               | Water                              | 1    | 285                       | 395                     |
| Adenosine triphosphate                  | Water                              | 1    | 285                       | 395                     |
| Adrenalin                               |                                    |      | 295                       | 335                     |
| <i>p</i> -Aminobenzoic acid             | Water                              | 8    | 295                       | 345                     |
| Aminopterin                             | Water                              | 7    | 280, 370                  | 460                     |
| 1-Aminopyrene                           | CF <sub>3</sub> COOH               |      | 330, 342                  | 415                     |
| <i>p</i> -Aminosalicylic acid           | Water                              | 11   | 300                       | 405                     |
| Amobarbital                             | Water                              | 14   | 265                       | 410                     |
| Anilines                                | Water                              | 7    | 280, 291                  | 344, 361                |
| Anthracene                              | Pentane                            |      | 420                       | 430                     |
| Anthranilic acid                        | Water                              | 7    | 300                       | 405                     |
| Azaindoles                              | Water                              | 10   | 290, 299                  | 310, 347                |
| Benz[ <i>c</i> ]acridine                | CF <sub>3</sub> COOH               |      | 295, 380                  | 480                     |
| Benz[ <i>a</i> ]anthracene              | Pentane                            |      | 284                       | 382                     |
| 1,2-Benzanthracene                      |                                    |      | 280, 340                  | 390, 410                |
| Benzanthrone                            | CF <sub>3</sub> COOH               |      | 370, 420                  | 550                     |
| Benzo[ <i>b</i> ]chrysene               | Pentane                            |      | 283                       | 398                     |
| 11- <i>H</i> -Benzo[ <i>a</i> ]fluorene | Pentane                            |      | 317                       | 340                     |
| Benzoic acid                            | 70% H <sub>2</sub> SO <sub>4</sub> |      | 285                       | 385                     |
| 3,4-Benzopyrene                         | Benzene                            |      | 365                       | 390, 480                |
| Benzo[ <i>e</i> ]pyrene                 | Pentane                            |      | 329                       | 389                     |
| Benzoquinoline                          | CF <sub>3</sub> COOH               |      | 280                       | 425                     |
| Benzoxanthane                           | Pentane                            |      | 363                       | 418                     |
| Bromolysergic acid diethyl amide        | Water                              | 1    | 315                       | 460                     |
| Brucine                                 | Water                              | 7    | 305                       | 500                     |
| Carbazole                               | <i>N,N</i> -Dimethyl formamide     |      | 291                       | 359                     |
| Chlortetracycline                       |                                    |      | 355                       | 445                     |
| Chrysene                                | Pentane                            |      | 250, 300, 310             | 260, 380                |
| Cinchonine                              | Water                              | 1    | 320                       | 420                     |
| Coumarin                                | Ethanol                            |      | 280                       | 352                     |
| Dibenzo[ <i>a,c</i> ]anthracene         | Pentane                            |      | 280                       | 381                     |
| Dibenzo[ <i>b,k</i> ]chrysene           | Pentane                            |      | 308                       | 428                     |
| Dibenzo[ <i>a,e</i> ]pyrene             | Pentane                            |      | 370                       | 401                     |
| 3,4,8,9-Dibenzopyrene                   |                                    |      | 370, 335, 390, 410        | 480, 510                |
| 5,12-Dihydronaphthacene                 | Pentane                            |      | 282                       | 340                     |
| 1,4-Diphenylbutadiene                   | Pentane                            |      | 328                       | 370                     |
| Epinephrine                             | Water                              | 7    | 295                       | 335                     |
| Ethacridine                             | Water                              | 2    | 370, 425                  | 515                     |
| Fluoranthrene                           | Pentane                            |      | 354                       | 464                     |
| Fluorene                                | Pentane                            |      | 300                       | 321                     |
| Fluorescein                             | Water                              | 7–11 | 490                       | 515                     |



**TABLE 7.16** Fluorescence Spectroscopy of Some Organic Compounds (*Continued*)

| Compound                            | Solvent                            | pH | Excitation wavelength, nm | Emission wavelength, nm |
|-------------------------------------|------------------------------------|----|---------------------------|-------------------------|
| Folic acid                          | Water                              | 7  | 365                       | 450                     |
| Gentisic acid                       | Water                              | 7  | 315                       | 440                     |
| Griseofulvin                        | Water                              | 7  | 295, 335                  | 450                     |
| Guanine                             | Water                              | 1  | 285                       | 365                     |
| Harmine                             | Water                              | 1  | 300, 365                  | 400                     |
| Hippuric acid                       | 70% H <sub>2</sub> SO <sub>4</sub> |    | 270                       | 370                     |
| Homovanillic acid                   | Water                              | 7  | 270                       | 315                     |
| <i>m</i> -Hydroxybenzoic acid       | Water                              | 12 | 314                       | 430                     |
| <i>p</i> -Hydroxycinnamic acid      | Water                              | 7  | 350                       | 440                     |
| 7-Hydroxycoumarin                   | Ethanol                            |    | 325                       | 441                     |
| 5-Hydroxyindole                     | Water                              | 1  | 290                       | 355                     |
| 5-Hydroxyindoleacetic acid          | Water                              | 7  | 300                       | 355                     |
| 3-Hydroxykynurenine                 | Water                              | 11 | 365                       | 460                     |
| <i>p</i> -Hydroxymandelic acid      | Water                              | 7  | 300                       | 380                     |
| <i>p</i> -Hydroxyphenylacetic acid  | Water                              | 7  | 280                       | 310                     |
| <i>p</i> -Hydroxyphenylpyruvic acid | Water                              | 7  | 290                       | 345                     |
| <i>p</i> -Hydroxyphenylserine       | Water                              | 1  | 290                       | 320                     |
| 5-Hydroxytryptophan                 | Water                              | 7  | 295                       | 340                     |
| Imipramine                          | Water                              | 14 | 295                       | 415                     |
| Indoleacetic acid                   | Water                              | 8  | 285                       | 360                     |
| Indoles                             | Water                              | 7  | 269, 315                  | 355                     |
| Indomethacin                        | Water                              | 13 | 300                       | 410                     |
| Kynurenine acid                     | Water                              | 7  | 325                       | 405                     |
|                                     |                                    | 11 | 325                       | 440                     |
| Lysergic acid diethylamide          | Water                              | 1  | 325                       | 445                     |
| Menadione                           | Ethanol                            |    | 335                       | 480                     |
| 9-Methylanthracene                  | Pentane                            |    | 382                       | 410                     |
| 3-Methylcholanthrene                | Pentane                            |    | 297                       | 392                     |
| 7-Methyldibenzopyrene               | Pentane                            |    | 460                       | 467                     |
| 2-Methylphenanthrene                | Pentane                            |    | 257                       | 357                     |
| 3-Methylphenanthrene                | Pentane                            |    | 292                       | 368                     |
| 1-Methylpyrene                      | Pentane                            |    | 336                       | 394                     |
| 4-Methylpyrene                      | Pentane                            |    | 338                       | 386                     |
| Naphthacene                         |                                    |    | 290, 310                  | 480, 515                |
| 1-Naphthol                          | 0.1 <i>M</i> NaOH                  |    | 365                       | 480                     |
|                                     | 20% ethanol                        |    |                           |                         |
| 2-Naphthol                          | 0.1 <i>M</i> NaOH                  |    | 365                       | 426                     |
|                                     | 20% ethanol                        |    |                           |                         |
| Oxytetracycline                     |                                    |    | 390                       | 520                     |
| Phenanthrene                        | Pentane                            |    | 252                       | 362                     |
| Phenylalanine                       | Water                              |    | 215, 260                  | 282                     |
| <i>o</i> -Phenylenepyrene           | Pentane                            |    | 360                       | 506                     |
| Phenylephrine                       |                                    |    | 270                       | 305                     |
| Picene                              | Pentane                            |    | 281                       | 398                     |
| Procaine                            | Water                              | 11 | 275                       | 345                     |
| Pyrene                              | Pentane                            |    | 330                       | 382                     |
| Pyridoxal                           | Water                              | 12 | 310                       | 365                     |
| Quinacrine                          | Water                              | 11 | 285                       | 420                     |
| Quinidine                           | Water                              | 1  | 350                       | 450                     |
| Quinine                             | Water                              | 1  | 250, 350                  | 450                     |
| Reserpine                           | Water                              | 1  | 300                       | 375                     |

**TABLE 7.16** Fluorescence Spectroscopy of Some Organic Compounds (*Continued*)

| Compound                       | Solvent        | pH | Excitation wavelength, nm | Emission wavelength, nm |
|--------------------------------|----------------|----|---------------------------|-------------------------|
| Resorcinol                     | Water          |    | 265                       | 315                     |
| Riboflavin                     | Water          | 7  | 270, 370, 445             | 520                     |
| Rutin                          | Water          | 1  | 430                       | 520                     |
| Salicyclic acid                | Water          | 11 | 310                       | 435                     |
| Scoparone                      | Water          | 10 | 350, 365                  | 430                     |
| Scopoletin                     | Water          | 10 | 365, 390                  | 460                     |
| Serotonin                      | 3 <i>M</i> HCl |    | 295                       | 550                     |
| Skatole                        | Water          |    | 290                       | 370                     |
| Streptomycin                   | Water          | 13 | 366                       | 445                     |
| <i>p</i> -Terphenyl            | Pentane        |    | 284                       | 338                     |
| Thiopental                     |                |    | 315                       | 530                     |
| Thymol                         | Water          | 7  | 265                       | 300                     |
| Tocopherol                     | Hexane-ethanol |    | 295                       | 340                     |
| Tribenzo[ <i>a,e,i</i> ]pyrene | Pentane        |    | 384                       | 448                     |
| Triphenylene                   | Pentane        |    | 288                       | 357                     |
| Tryptamine                     | Water          | 7  | 290                       | 360                     |
| Tryptophan                     | Water          | 11 | 285                       | 365                     |
| Tyramine                       | Water          | 1  | 275                       | 310                     |
| Tyrosine                       | Water          | 7  | 275                       | 310                     |
| Uric acid                      | Water          | 1  | 325                       | 370                     |
| Vitamin A                      | 1-Butanol      |    | 340                       | 490                     |
| Vitamin B <sub>12</sub>        | Water          | 7  | 275                       | 305                     |
| Warfarin                       | Methanol       |    | 290, 342                  | 385                     |
| Xanthine                       | Water          | 1  | 315                       | 435                     |
| 2,6-Xylenol                    |                |    | 275                       | 305                     |
| 3,4-Xylenol                    |                |    | 280                       | 310                     |
| Yohimbine                      | Water          | 1  | 270                       | 360                     |
| Zoxazolamine                   | Water          | 11 | 280                       | 320                     |

TABLE 7.17 Fluorescence Quantum Yield Values

| Compound                      | Solvent                           | $Q_F$ value vs. $Q_F$ standard          |
|-------------------------------|-----------------------------------|-----------------------------------------|
| $Q_F$ standard                |                                   |                                         |
| 9-Aminoacridine               | Water                             | 0.99                                    |
| Anthracene                    | Ethanol                           | 0.30                                    |
| POPOP*                        | Toluene                           | 0.85                                    |
| Quinine sulfate dihydrate     | 1N H <sub>2</sub> SO <sub>4</sub> | 0.55                                    |
| Secondary standards           |                                   |                                         |
| Acridine orange hydrochloride | Ethanol                           | 0.54 Quinine sulfate<br>0.58 Anthracene |
| 1,8-ANS† (free acid)          | Ethanol                           | 0.38 Anthracene<br>0.39 POPOP           |
| 1,8-ANS (magnesium salt)      | Ethanol                           | 0.29 Anthracene<br>0.31 POPOP           |
| Fluorescein                   | 0.1N NaOH                         | 0.91 Quinine sulfate<br>0.94 POPOP      |
| Fluorescein, ethyl ester      | 0.1N NaOH                         | 0.99 Quinine sulfate<br>0.99 POPOP      |
| Rhodamine B                   | Ethanol                           | 0.69 Quinine sulfate<br>0.70 Anthracene |
| 2,6-TNS‡ (potassium salt)     | Ethanol                           | 0.48 Anthracene<br>0.51 POPOP           |

\* POPOP *p*-bis[2-(5-phenyloxazolyl)]benzene.  
† ANS, anilino-8-naphthalene sulfonic acid.  
‡ TNS, 2-*p*-toluidinylnaphthalene-6-sulfonate.

7.4 FLAME ATOMIC EMISSION, FLAME ATOMIC  
ABSORPTION, ELECTROTHERMAL (FURNACE)  
ATOMIC ABSORPTION, ARGON INDUCTION  
COUPLED PLASMA, AND PLASMA ATOMIC  
FLUORESCENCE

The tables of atomic emission and atomic absorption lines are presented in two parts. In Table 7.18 the data are arranged in alphabetic order by name of the element, whereas in Table 7.19 the sensitive lines of the elements are arranged in order of decreasing wavelengths. For additional lines and their relative intensities consult W. F. Meggers, C. H. Corliss, and B. F. Scribner, *Tables of Spectral-Line Intensities, Part I*, National Bureau of Standards Monograph 32, U.S. Government Printing Office, Washington, D.C., 1961.

The detection limits in the table correspond generally to the concentration of an element required to give a net signal equal to three times the standard deviation of the noise (background) in accordance with IUPAC recommendations. Detection limits can be confusing when steady-state techniques such as flame atomic emission or absorption, and plasma atomic emission or fluorescence, which

**TABLE 7.18** Detection Limits in ng/mL

The detection limits in the table correspond generally to the concentration of analyte required to give a net signal equal to three times the standard deviation of the background in accordance with IUPAC recommendations.

| Element               | Wavelength,<br>nm | Flame<br>emission | Flame<br>atomic<br>absorption | Electrothermal<br>atomic<br>absorption | Argon<br>ICP | Plasma<br>atomic<br>fluorescence |
|-----------------------|-------------------|-------------------|-------------------------------|----------------------------------------|--------------|----------------------------------|
| Aluminum              | 308.22            |                   | 40                            |                                        | 10           |                                  |
|                       | 309.28            |                   | 20                            | 0.05                                   | 11           | 4                                |
|                       | 394.40            | 3.6               | 45                            |                                        | 36           |                                  |
|                       | 396.15            | 7.5               | 30                            | 0.01                                   | 20           | 5                                |
| Antimony              | 206.83            |                   |                               |                                        | 50           |                                  |
|                       | 217.58            |                   | 30                            |                                        | 50           |                                  |
|                       | 231.15            | 70                |                               |                                        | 30           | 10                               |
|                       | 259.81            | 200               |                               | 0.08                                   |              | 0.1                              |
| Arsenic               | 189.04            |                   | 160                           |                                        | 35           |                                  |
|                       | 193.76            |                   | 120                           | 1                                      | 50           |                                  |
|                       | 197.20            |                   | 240                           |                                        |              |                                  |
|                       | 228.81            | 455               |                               |                                        |              |                                  |
| Barium                | 234.90            | 250               |                               |                                        |              | 10                               |
|                       | 455.36            | 3                 |                               |                                        | 0.9          |                                  |
|                       | 493.41            | 4                 |                               |                                        | 1            |                                  |
|                       | 553.55            | 1.5               | 9                             | 0.04                                   |              | 2                                |
| Beryllium             | 234.86            |                   | 1                             | 0.05                                   | 0.4          |                                  |
|                       | 313.04            |                   | 2                             | 0.003                                  | 1            |                                  |
|                       | 313.11            | 100               |                               |                                        | 1            | 0.2                              |
|                       | 223.06            |                   | 18                            | 0.35                                   | 30           |                                  |
| Bismuth               | 227.66            |                   |                               | 2                                      |              |                                  |
|                       | 306.77            | 60                |                               | 0.5                                    | 30           | 2                                |
|                       | 182.59            |                   |                               |                                        | 8            |                                  |
|                       | 249.77            |                   | 700                           | 15                                     | 3            | 60                               |
| (as BO <sub>2</sub> ) | 518.0             | 50                |                               |                                        |              |                                  |
| (as BO <sub>2</sub> ) | 547.6             | 50                |                               |                                        |              |                                  |
| Bromine               | 154.07            |                   |                               |                                        | 50           |                                  |
| Cadmium               | 214.44            |                   |                               |                                        | 1.0          |                                  |
|                       | 226.50            |                   |                               |                                        | 0.6          |                                  |
|                       | 228.80            | 6                 | 1                             | 0.008                                  | 228          |                                  |
|                       | 326.11            | 3                 | 0.5                           | 0.014                                  |              | 0.001                            |
| Calcium               | 315.89            |                   |                               |                                        | 20           |                                  |
|                       | 393.37            |                   |                               |                                        | 0.6          |                                  |
|                       | 396.85            |                   |                               |                                        | 1.2          |                                  |
|                       | 422.67            | 1.5               | 1                             | 0.3                                    |              | 0.08                             |
| Carbon                | 193.09            |                   |                               |                                        | 44           |                                  |
|                       | 247.86            |                   |                               |                                        | 1000         |                                  |
| Cerium                | 413.38            |                   |                               |                                        | 30           |                                  |
|                       | 418.66            |                   |                               |                                        | 30           |                                  |
|                       | 569.92            | 150               |                               |                                        |              |                                  |
| Cesium                | 852.11            | 0.02              | 8                             | 0.04                                   |              |                                  |
|                       | 894.35            | 0.04              | 130                           |                                        |              |                                  |
| Chlorine              | 134.72            |                   |                               |                                        | 50           |                                  |
| Chromium              | 267.72            |                   |                               |                                        | 3            |                                  |
|                       | 283.58            |                   |                               |                                        | 20           |                                  |
|                       | 284.98            |                   |                               |                                        | 30           |                                  |
|                       | 357.87            | 6                 | 2                             | 0.05                                   |              | 0.4                              |
|                       | 359.35            | 7                 |                               |                                        |              |                                  |
|                       |                   |                   |                               |                                        |              |                                  |

**TABLE 7.18** Detection Limits in ng/mL (*Continued*)

| Element                    | Wavelength,<br>nm | Flame<br>emission | Flame<br>atomic<br>absorption | Electrothermal<br>atomic<br>absorption | Argon<br>ICP | Plasma<br>atomic<br>fluorescence |
|----------------------------|-------------------|-------------------|-------------------------------|----------------------------------------|--------------|----------------------------------|
| Chromium<br><i>(cont.)</i> | 360.53            | 13                |                               |                                        |              |                                  |
|                            | 425.44            | 3                 | 6                             |                                        | 66           |                                  |
|                            | 427.48            | 4                 |                               |                                        |              |                                  |
|                            | 428.97            | 5                 |                               |                                        |              |                                  |
| Cobalt                     | 228.62            |                   |                               |                                        | 3            |                                  |
|                            | 238.89            |                   |                               |                                        | 28           |                                  |
|                            | 240.73            | 5                 | 8                             | 0.01                                   | 7            | 0.4                              |
|                            | 345.35            | 30                |                               |                                        |              |                                  |
| Copper                     | 324.75            | 1.5               | 1                             | 0.01                                   | 2            | 0.2                              |
|                            | 327.40            | 3                 | 2                             | 0.02                                   | 4            |                                  |
| Dysprosium                 | 353.17            |                   |                               |                                        | 3            |                                  |
|                            | 340.78            |                   |                               |                                        | 6            |                                  |
|                            | 404.60            | 30                | 50                            |                                        |              | 300                              |
|                            | 418.68            |                   | 60                            |                                        |              |                                  |
| Erbium                     | 421.17            |                   | 60                            |                                        |              |                                  |
|                            | 323.06            |                   |                               |                                        | 15           |                                  |
|                            | 349.81            |                   |                               |                                        | 10           |                                  |
|                            | 400.80            | 30                | 40                            | 0.3                                    |              | 500                              |
| Europium                   | 408.77            |                   | 40                            |                                        |              |                                  |
|                            | 381.97            |                   |                               |                                        | 2            |                                  |
|                            | 412.97            |                   |                               |                                        | 3            |                                  |
| Gadolinium                 | 459.40            | 0.45              | 20                            | 0.5                                    |              | 20                               |
|                            | 335.05            |                   |                               |                                        | 10           |                                  |
|                            | 368.41            |                   | 4000                          |                                        |              |                                  |
| Gallium                    | 440.19            | 72                | 1000                          | 8                                      |              | 800                              |
|                            | 287.42            |                   | 70                            |                                        |              |                                  |
|                            | 294.36            |                   | 20                            |                                        | 30           |                                  |
|                            | 404.30            | 5                 | 50                            |                                        |              |                                  |
| Germanium                  | 417.21            | 3                 | 30                            | 1                                      | 40           | 0.9                              |
|                            | 209.43            |                   |                               |                                        | 50           |                                  |
|                            | 219.87            |                   |                               |                                        | 100          |                                  |
|                            | 265.12            | 400               | 40                            | 7.5                                    |              | 50                               |
| Gold                       | 242.80            |                   | 10                            | 0.5                                    | 5            |                                  |
|                            | 267.60            | 500               | 8                             | 0.5                                    | 10           | 0.3                              |
| Hafnium                    | 263.87            |                   |                               |                                        | 10           |                                  |
|                            | 277.34            |                   |                               |                                        | 10           |                                  |
|                            | 307.29            |                   | 2000                          |                                        |              |                                  |
|                            | 339.90            |                   |                               |                                        | 3            |                                  |
| Holmium                    | 345.60            |                   |                               |                                        | 8            |                                  |
|                            | 405.39            | 15                | 40                            | 0.7                                    |              | 100                              |
|                            | 410.38            |                   | 30                            |                                        |              |                                  |
|                            | 230.61            |                   |                               |                                        | 40           |                                  |
| Indium                     | 303.94            | 100               | 7                             | 0.01                                   |              |                                  |
|                            | 325.61            | 22                | 8                             |                                        |              |                                  |
|                            | 410.18            | 14                | 20                            |                                        |              |                                  |
|                            | 451.13            | 0.7               | 22                            |                                        | 2            | 0.2                              |
| Iodine                     | 178.38            |                   |                               |                                        | 20           |                                  |
|                            | 183.0             |                   |                               | 3                                      |              |                                  |
| Iridium                    | 208.88            | 400               | 500                           | 0.5                                    |              |                                  |
|                            | 212.68            |                   |                               |                                        | 20           |                                  |
|                            | 224.27            |                   |                               |                                        | 20           |                                  |

**TABLE 7.18** Detection Limits in ng/mL (*Continued*)

| Element    | Wavelength,<br>nm | Flame<br>emission | Flame<br>atomic<br>absorption | Electrothermal<br>atomic<br>absorption | Argon<br>ICP | Plasma<br>atomic<br>fluorescence |
|------------|-------------------|-------------------|-------------------------------|----------------------------------------|--------------|----------------------------------|
| Iron       | 238.20            |                   |                               |                                        | 4            |                                  |
|            | 248.33            |                   | 3                             | 0.01                                   |              |                                  |
|            | 259.94            |                   |                               |                                        | 3            |                                  |
|            | 302.06            | 18                | 5                             |                                        |              |                                  |
|            | 371.99            | 15                | 10                            |                                        |              | 0.3                              |
| Lanthanum  | 385.99            | 12                | 21                            |                                        |              |                                  |
|            | 379.48            |                   |                               |                                        | 15           |                                  |
|            | 392.76            |                   | 8000                          |                                        |              |                                  |
|            | 408.67            |                   |                               |                                        | 2            |                                  |
|            | 550.13            | 20                |                               |                                        |              |                                  |
| (as LaO)   | 579.13            | 5                 | 2000                          | 0.5                                    |              |                                  |
|            | 441.82            | 100               |                               |                                        |              |                                  |
|            | 560.25            | 300               |                               |                                        |              |                                  |
| Lead       | 217.10            |                   | 20                            | 0.4                                    |              |                                  |
|            | 220.35            |                   |                               |                                        | 20           |                                  |
|            | 283.31            | 60                | 10                            | 1                                      |              | 5                                |
|            | 368.35            | 30                |                               |                                        |              |                                  |
|            | 405.78            | 20                |                               |                                        |              |                                  |
| Lithium    | 460.29            | 0.06              | 30                            |                                        | 50           |                                  |
|            | 610.36            | 0.001             |                               |                                        |              |                                  |
|            | 670.78            | 0.003             | 0.3                           | 1.5                                    | 5            | 0.4                              |
| Lutetium   | 261.54            |                   |                               |                                        | 1            |                                  |
|            | 307.76            |                   |                               |                                        | 6            |                                  |
| Magnesium  | 279.08            |                   |                               |                                        | 30           |                                  |
|            | 279.55            |                   |                               |                                        | 1.5          |                                  |
|            | 285.21            | 4.5               | 0.1                           | 0.018                                  | 3.6          | 0.4                              |
| Manganese  | 256.37            |                   |                               |                                        | 2.7          |                                  |
|            | 257.61            |                   |                               |                                        | 0.5          |                                  |
|            | 259.37            |                   | 60                            |                                        | 3            |                                  |
|            | 260.57            |                   |                               |                                        | 6            |                                  |
|            | 279.48            | 1                 | 1                             | 0.05                                   |              | 0.4                              |
|            | 293.30            |                   |                               |                                        | 24           |                                  |
|            | 294.92            |                   |                               |                                        | 24           |                                  |
| Mercury    | 403.08            | 1.5               | 30                            |                                        |              |                                  |
|            | 194.23            |                   |                               |                                        | 30           |                                  |
|            | 253.65            | 150               | 0.001                         | 6                                      | 50           | 5                                |
| Molybdenum | 202.03            |                   |                               |                                        | 5            |                                  |
|            | 203.84            |                   |                               |                                        | 8            |                                  |
|            | 281.62            |                   |                               |                                        | 1.2          |                                  |
|            | 313.26            | 220               | 30                            | 0.06                                   |              | 12                               |
|            | 390.30            | 75                | 50                            |                                        |              |                                  |
| Neodymium  | 292.45            | 200               |                               |                                        |              |                                  |
|            | 401.23            |                   |                               |                                        | 10           |                                  |
|            | 430.36            |                   |                               |                                        | 30           |                                  |
|            | 492.45            | 150               | 600                           |                                        |              | 2000                             |
| Nickel     | 231.60            |                   |                               |                                        | 6            |                                  |
|            | 232.00            | 8                 | 4                             | 0.5                                    | 10           |                                  |
|            | 341.48            | 15                | 2                             |                                        |              |                                  |
|            | 352.45            | 8                 | 2                             |                                        |              | 2                                |
| Niobium    | 316.34            |                   |                               |                                        | 20           |                                  |
|            | 405.89            | 250               | 1000                          |                                        |              | 1000                             |

**TABLE 7.18** Detection Limits in ng/mL (*Continued*)

| Element                        | Wavelength,<br>nm | Flame<br>emission | Flame<br>atomic<br>absorption | Electrothermal<br>atomic<br>absorption | Argon<br>ICP | Plasma<br>atomic<br>fluorescence |
|--------------------------------|-------------------|-------------------|-------------------------------|----------------------------------------|--------------|----------------------------------|
| Osmium                         | 225.58            |                   |                               |                                        | 20           |                                  |
|                                | 228.23            |                   |                               |                                        | 40           |                                  |
|                                | 263.71            | 2000              | 80                            |                                        |              |                                  |
|                                | 290.91            |                   | 110                           |                                        |              |                                  |
| Palladium                      | 244.8             | 20                | 20                            | 0.5                                    |              | 40                               |
|                                | 340.46            | 25                | 80                            |                                        | 40           |                                  |
|                                | 363.47            | 50                |                               |                                        | 60           |                                  |
| Phosphorus<br>(as HPO)         | 178.28            |                   |                               |                                        | 50           |                                  |
|                                | 213.62            |                   |                               |                                        | 50           |                                  |
|                                | 524.9             | 100               |                               |                                        |              |                                  |
| Platinum                       | 214.42            |                   |                               |                                        | 20           |                                  |
|                                | 265.95            | 2000              | 100                           | 0.2                                    | 40           | 300                              |
| Potassium                      | 404.41            | 1.3               | 100                           |                                        |              |                                  |
|                                | 404.72            | 2.6               |                               |                                        |              |                                  |
|                                | 766.49            | 0.15              | 1                             | 0.004                                  | 200          | 0.6                              |
|                                | 769.90            | 0.3               | 2                             |                                        |              |                                  |
| Praseodymium                   | 390.84            |                   |                               |                                        | 20           |                                  |
|                                | 414.31            |                   |                               |                                        | 30           |                                  |
|                                | 493.97            | 300               |                               |                                        |              | 1000                             |
| Rhenium                        | 197.31            |                   |                               |                                        | 8            |                                  |
|                                | 345.19            | 690               |                               |                                        |              |                                  |
|                                | 346.05            | 200               | 200                           | 10                                     |              |                                  |
|                                | 346.47            | 275               |                               |                                        |              |                                  |
| Rhodium                        | 343.49            | 10                | 2                             | 0.1                                    | 20           | 100                              |
|                                | 369.24            | 20                |                               |                                        | 30           |                                  |
| Rubidium                       | 780.02            | 0.0065            | 0.3                           |                                        | 500          | 3                                |
|                                | 794.76            | 0.013             |                               |                                        |              |                                  |
| Ruthenium                      | 240.27            |                   |                               |                                        | 50           |                                  |
|                                | 349.89            | 80                | 70                            | 10                                     | 150          | 500                              |
|                                | 442.43            |                   |                               |                                        | 10           |                                  |
| Samarium                       | 476.03            | 30                | 500                           |                                        | 100          |                                  |
|                                | 255.24            |                   |                               |                                        | 21           |                                  |
| Scandium                       | 357.24            |                   |                               |                                        | 1            |                                  |
|                                | 361.38            |                   |                               |                                        | 1.5          |                                  |
|                                | 391.18            | 21                | 20                            | 6                                      | 120          | 10                               |
|                                | 402.04            | 30                |                               |                                        |              |                                  |
|                                | 402.34            | 30                |                               |                                        |              |                                  |
|                                | 196.03            |                   | 90                            | 2.5                                    | 6            | 10                               |
| Selenium                       | 251.61            |                   | 80                            | 0.5                                    | 10           | 50                               |
| Silver                         | 283.16            |                   |                               |                                        | 15           |                                  |
|                                | 328.07            | 2                 | 0.9                           | 0.001                                  | 4.5          | 0.1                              |
|                                | 338.29            | 4                 |                               |                                        | 3            |                                  |
| Sodium                         | 330.23            | 125               |                               | 0.7                                    | 15           |                                  |
|                                | 330.30            | 250               |                               |                                        |              |                                  |
|                                | 589.00            | 0.01              | 0.2                           | 0.004                                  | 20           | 0.2                              |
| Strontium                      | 589.59            | 0.02              |                               |                                        |              |                                  |
|                                | 407.78            |                   |                               |                                        | 1            |                                  |
|                                | 421.55            |                   |                               |                                        | 0.5          |                                  |
|                                | 460.73            | 0.1               | 2                             | 0.01                                   |              | 0.3                              |
| Sulfur<br>(as S <sub>2</sub> ) | 180.73            |                   | 10                            |                                        | 70           |                                  |
|                                | 394.0             | 1600              |                               |                                        |              |                                  |

**TABLE 7.18** Detection Limits in ng/mL (*Continued*)

| Element   | Wavelength,<br>nm                                        | Flame<br>emission | Flame<br>atomic<br>absorption | Electrothermal<br>atomic<br>absorption | Argon<br>ICP | Plasma<br>atomic<br>fluorescence |
|-----------|----------------------------------------------------------|-------------------|-------------------------------|----------------------------------------|--------------|----------------------------------|
| Tantalum  | 240.06<br>271.47                                         |                   | 800                           |                                        | 20           |                                  |
| Tellurium | 214.27<br>238.58                                         | 150               | 15                            | 0.5                                    | 60           | 2                                |
| Terbium   | 350.92<br>384.87                                         |                   |                               |                                        | 10<br>40     |                                  |
| Thallium  | 431.89<br>190.86<br>276.78<br>351.92<br>377.57<br>535.0  | 150               | 600                           |                                        | 50<br>150    | 500                              |
| Thorium   | 283.73<br>401.91                                         |                   | 9                             | 0.15                                   |              |                                  |
| Thulium   | 313.13<br>371.79<br>384.80                               |                   |                               |                                        |              |                                  |
| Tin       | 189.99<br>224.60<br>284.00<br>286.33                     | 3<br>1.5          |                               | 0.5                                    |              | 4                                |
| Titanium  | 334.19<br>334.94<br>337.28<br>364.27<br>365.35<br>399.86 | 4                 | 10                            |                                        |              |                                  |
| Tungsten  | 207.91<br>209.48<br>400.87                               |                   |                               |                                        |              |                                  |
| Uranium   | 358.49<br>385.96<br>409.01                               | 100               | 110<br>200<br>160             | 1<br>1.5                               | 30           | 10                               |
| Vanadium  | 292.40<br>310.23<br>318.34<br>318.54<br>437.92           | 400               | 60                            | 2.5                                    | 6<br>8       | 30                               |
| Ytterbium | 328.94<br>369.42<br>398.80                               |                   |                               |                                        |              |                                  |
| Yttrium   | 360.07<br>362.09<br>371.03<br>410.24                     |                   |                               |                                        |              |                                  |
| Zinc      | 202.55<br>213.86                                         |                   |                               |                                        |              |                                  |
| Zirconium | 339.20<br>343.82<br>349.62<br>360.12                     |                   |                               |                                        |              |                                  |



TABLE 7.19 Sensitive Lines of the Elements

In this table the sensitive lines of the elements are arranged in order of decreasing wavelengths. A Roman numeral II following an element designation indicates a line classified as being emitted by the singly ionized atom. In the column headed Sensitivity, the most sensitive line of the non-ionized atom is indicated by U1, and other lines by U2, U3, and so on, in order of decreasing sensitivity. For the singly ionized atom the corresponding designations are V1, V2, V3, and so on.

| Wavelength, nm | Element | Sensitivity | Wavelength, nm | Element | Sensitivity |
|----------------|---------|-------------|----------------|---------|-------------|
| 894.35         | Cs      | U2          | 492.45         | Nd      | U1          |
| 852.11         | Cs      | U1          | 488.91         | Re      | U4          |
| 819.48         | Na      | U4          | 487.25         | Sr      | U3          |
| 818.33         | Na      | U3          | 483.21         | Sr      | U2          |
| 811.53         | Ar      | U2          | 482.59         | Ra      | U1          |
| 794.76         | Rb      | U2          | 481.95         | Cl II   | V4          |
| 780.02         | Rb      | U1          | 481.67         | Br II   | V3          |
| 769.90         | K       | U2          | 481.05         | Zn      | U3          |
| 766.49         | K       | U1          | 481.01         | Cl II   | V3          |
| 750.04         | Ar      | U4          | 479.45         | Cl II   | V2          |
| 706.72         | Ar      | U3          | 478.55         | Br II   | V2          |
| 696.53         | Ar      | U3          | 476.03         | Sm      | U1          |
| 690.24         | F       | U3          | 470.09         | Br II   | V1          |
| 685.60         | F       | U2          | 467.12         | Xe      | U2          |
| 670.78         | Li      | U1          | 462.43         | Xe      | U3          |
| 656.28         | H       | U2          | 460.73         | Sr      | U1          |
| 649.69         | Ba II   | V4          | 460.29         | Li      | U4          |
| 624.99         | La      | U3          | 459.40         | Eu      | U1          |
| 614.17         | Ba II   | V3          | 459.32         | Cs      | U4          |
| 610.36         | Li      | U2          | 455.54         | Cs      | U3          |
| 593.06         | La      | U4          | 455.40         | Ba II   | V1          |
| 589.59         | Na      | U2          | 451.13         | In      | U1          |
| 589.00         | Na      | U1          | 450.10         | Xe      | U4          |
| 587.76         | He      | U3          | 445.48         | Ca      | U2          |
| 587.09         | Kr      | U2          | 442.43         | Sm II   | V4          |
| 579.13         | La      | U1          | 440.85         | V       | U4          |
| 569.92         | Ce      | U1          | 440.19         | Gd      | U1          |
| 567.96         | N II    | V2          | 439.00         | V       | U3          |
| 567.60         | N II    | V4          | 437.49         | Y II    | V4          |
| 566.66         | N II    | V3          | 437.92         | V       | U1          |
| 557.02         | Kr      | U3          | 435.84         | Hg      | U3          |
| 553.55         | Ba      | U1          | 431.89         | Tb      | U1          |
| 550.13         | La      | U2          | 430.36         | Nd II   | V2          |
| 546.55         | Ag      | U4          | 430.21         | W       | U1          |
| 546.07         | Hg      | U2          | 429.67         | Sm      | U1          |
| 545.52         | La      | U3          | 428.97         | Cr      | U3          |
| 535.84         | Hg      | U3          | 427.48         | Cr      | U2          |
| 535.05         | Tl      | U1          | 425.43         | Cr      | U1          |
| 521.82         | Cu      | U3          | 422.67         | Ca      | U1          |
| 520.91         | Ag      | U3          | 421.56         | Rb      | U4          |
| 520.84         | Cr      | U8          | 421.55         | Sr II   | V1          |
| 520.60         | Cr      | U7          | 421.17         | Dy      | U2          |
| 515.32         | Cu      | U4          | 420.19         | Rb      | U3          |
| 498.18         | Ti      | U1          | 418.68         | Dy      | U2          |
| 496.23         | Sr      | U2          | 418.66         | Ce II   | V1          |
| 493.97         | Pr      | U1          | 417.21         | Ga      | U1          |
| 493.41         | Ba II   | V2          | 414.31         | Pr II   | V2          |

**TABLE 7.19** Sensitive Lines of the Elements (*Continued*)

| Wavelength, nm | Element | Sensitivity | Wavelength, nm | Element | Sensitivity |
|----------------|---------|-------------|----------------|---------|-------------|
| 414.29         | Y       | U4          | 386.41         | Mo      | U2          |
| 413.38         | Ce II   | V1          | 385.99         | Fe      | U2          |
| 413.07         | Ba II   | V5          | 385.96         | U II    | V1          |
| 412.97         | Eu II   | V2          | 384.87         | Tb II   | V2          |
| 412.83         | Y       | U3          | 384.80         | Tm II   | V2          |
| 412.38         | Nb      | U4          | 383.83         | Mg      | U2          |
| 412.32         | La II   | V4          | 383.82         | Mo      | U2          |
| 411.00         | N       | U2          | 382.23         | Mg      | U3          |
| 410.38         | Ho      | U1          | 382.94         | Mg      | U4          |
| 410.24         | Y       | U1          | 381.97         | Eu II   | V1          |
| 410.18         | In      | U2          | 379.94         | Ru      | U3          |
| 410.09         | Nb      | U3          | 379.63         | Mo      | U1          |
| 409.99         | N       | U3          | 379.48         | La II   | V2          |
| 409.01         | U II    | V2          | 379.08         | La II   | V3          |
| 408.77         | Er      | U1          | 377.57         | Tl      | U3          |
| 408.67         | La II   | V1          | 377.43         | Y II    | V3          |
| 407.97         | Nb      | U2          | 374.83         | Fe      | U4          |
| 407.77         | Sr II   | V2          | 373.49         | Fe      | U2          |
| 407.74         | Y       | U2          | 372.80         | Ru      | U1          |
| 407.74         | La II   | V2          | 371.99         | Fe      | U1          |
| 407.43         | W       | U2          | 371.79         | Tm      | U1          |
| 405.89         | Nb      | U1          | 371.03         | Y II    | V1          |
| 405.78         | Pb      | U1          | 369.42         | Yb II   | V2          |
| 405.39         | Ho      | U2          | 369.24         | Rh      | U2          |
| 404.72         | K       | U4          | 368.41         | Gd      | U2          |
| 404.66         | Hg      | U5          | 368.35         | Pb      | U2          |
| 404.60         | Dy      | U1          | 365.48         | Hg      | U4          |
| 404.41         | K       | U3          | 365.35         | Ti      | U2          |
| 403.45         | Mn      | U3          | 365.01         | Hg      | U3          |
| 403.31         | Mn      | U2          | 364.28         | Sc II   | V3          |
| 403.30         | Ga      | U2          | 364.27         | Sn      | U3          |
| 403.08         | Mn      | U1          | 363.47         | Pd      | U2          |
| 402.37         | Sc      | U3          | 363.07         | Sc II   | V2          |
| 402.04         | Sc      | U3          | 362.09         | Y       | U2          |
| 401.91         | Th II   | V1          | 361.38         | Sc II   | V1          |
| 401.23         | Nd II   | V1          | 360.96         | Pd      | U2          |
| 400.87         | W       | U1          | 360.12         | Zr      | U1          |
| 400.80         | Er      | U1          | 360.07         | Y II    | V2          |
| 399.86         | Cr      | U1          | 360.05         | Cr      | U6          |
| 399.86         | Ti      | U1          | 359.62         | Ru      | U3          |
| 398.80         | Yb      | U1          | 359.34         | Cr      | U5          |
| 396.85         | Ca II   | V2          | 359.26         | Sm II   | V1          |
| 396.15         | Al      | U1          | 358.49         | U       | V1          |
| 394.91         | La II   | V2          | 357.87         | Cr      | U4          |
| 394.40         | Al      | U2          | 357.25         | Zr II   | V4          |
| 393.37         | Ca II   | V1          | 357.24         | Sc II   | V1          |
| 391.18         | Sc      | U1          | 356.83         | Sn II   | V1          |
| 390.84         | Pr II   | V1          | 355.31         | Pd      | U3          |
| 390.75         | Sc      | U2          | 354.77         | Zr      | U3          |
| 390.30         | Mo      | U1          | 353.17         | Dy II   | V1          |
| 389.18         | Ba      | V4          | 352.98         | Co      | U3          |
| 388.86         | He      | U2          | 352.94         | Tl      | U4          |
| 388.63         | Fe      | U5          | 352.69         | Co      | U4          |

TABLE 7.19 Sensitive Lines of the Elements (Continued)

| Wavelength, nm | Element | Sensitivity | Wavelength, nm | Element | Sensitivity |
|----------------|---------|-------------|----------------|---------|-------------|
| 352.45         | Ni      | U2          | 324.75         | Cu      | U1          |
| 351.96         | Zr      | U3          | 324.27         | Pd      | U4          |
| 351.92         | Tl      | U2          | 323.45         | Cr      | V3          |
| 351.69         | Pd      | U3          | 323.26         | Li      | U3          |
| 351.36         | Ir      | U2          | 323.06         | Er II   | V2          |
| 350.92         | Tb II   | V1          | 322.08         | Ir      | U1          |
| 350.63         | Co      | U3          | 318.54         | V       | U3          |
| 350.23         | Co      | U2          | 318.40         | V       | U2          |
| 349.89         | Ru      | U2          | 317.93         | Ca II   | V3          |
| 349.62         | Zr II   | V3          | 316.34         | Nb II   | V1          |
| 349.41         | Er II   | V1          | 315.89         | Ca II   | V4          |
| 348.11         | Pd      | U5          | 313.26         | Mo      | U2          |
| 347.40         | Ni      | U3          | 313.13         | Tm II   | V1          |
| 346.47         | Re      | U2          | 313.11         | Be      | U1          |
| 346.05         | Re      | U1          | 313.04         | Be      | U2          |
| 345.60         | Ho II   | V2          | 311.84         | V II    | V4          |
| 345.58         | Co      | U5          | 311.07         | V II    | V3          |
| 345.19         | Re      | U3          | 310.23         | V II    | V2          |
| 345.14         | B II    | V2          | 309.42         | Nb II   | V1          |
| 344.36         | Co      | U2          | 309.31         | V II    | V1          |
| 344.06         | Fe      | U2          | 309.27         | Al      | U3          |
| 343.82         | Zr II   | V2          | 308.22         | Al      | U4          |
| 343.67         | Ru      | U2          | 307.76         | Lu II   | V2          |
| 343.49         | Rh      | U1          | 307.29         | Hf      | U1          |
| 342.83         | Ru      | U4          | 306.77         | Bi      | U3          |
| 342.12         | Pd      | U3          | 306.47         | Pt      | U1          |
| 341.48         | Ni      | U3          | 303.94         | In      | U4          |
| 341.23         | Co      | U4          | 303.90         | Ge      | U2          |
| 340.78         | Dy II   | V2          | 303.41         | Sn      | U3          |
| 340.51         | Co      | U2          | 302.06         | Fe      | U3          |
| 340.46         | Pd      | U2          | 300.91         | Sn      | U4          |
| 339.90         | Ho II   | V1          | 294.91         | Mn II   | V4          |
| 339.20         | Zr II   | V1          | 294.44         | W       | U5          |
| 338.29         | Ag      | U2          | 294.36         | Ga      | U3          |
| 337.28         | Ti II   | V3          | 294.02         | Ta      | U3          |
| 336.12         | Ti II   | V2          | 293.30         | Mn II   | V4          |
| 335.05         | Gd II   | V1          | 292.98         | Pt      | U3          |
| 334.94         | Ti II   | V1          | 292.45         | Nd      | U2          |
| 334.50         | Zn      | U2          | 292.40         | V II    | V1          |
| 334.19         | Ti      | U4          | 290.91         | Os      | U2          |
| 332.11         | Be      | U3          | 289.80         | Bi      | U2          |
| 331.12         | Ta      | U3          | 289.10         | Mo II   | V4          |
| 330.03         | Na      | U6          | 288.16         | Si      | U1          |
| 330.26         | Zn      | U3          | 287.42         | Ga      | U4          |
| 330.23         | Na      | U5          | 287.15         | Mo II   | V3          |
| 328.94         | Yb II   | V1          | 286.33         | Sn      | U2          |
| 328.23         | Zn      | U5          | 286.04         | As      | U2          |
| 328.07         | Ag      | U1          | 285.21         | Mg      | U1          |
| 327.40         | Cu      | U2          | 284.82         | Mo II   | V2          |
| 326.95         | Ge      | U3          | 284.00         | Sn      | U1          |
| 326.23         | Sn      | U3          | 283.73         | Th II   | V1          |
| 326.11         | Cd      | U1          | 283.58         | Cr II   | V2          |
| 325.61         | In      | U3          | 283.31         | Pb      | U3          |

**TABLE 7.19** Sensitive Lines of the Elements (*Continued*)

| Wavelength, nm | Element | Sensitivity | Wavelength, nm | Element | Sensitivity |
|----------------|---------|-------------|----------------|---------|-------------|
| 283.16         | Si II   | V1          | 239.56         | Fe II   | V2          |
| 283.03         | Pt      | U3          | 238.89         | Co II   | V2          |
| 281.62         | Al II   | V2          | 238.58         | Te      | U2          |
| 281.61         | Mo II   | V1          | 238.32         | Te      | U3          |
| 280.27         | Mg II   | V2          | 238.20         | Fe II   | V1          |
| 280.20         | Pb      | U4          | 234.90         | As      | U4          |
| 279.83         | Mn      | U3          | 234.86         | Be      | U1          |
| 279.55         | Mg II   | V1          | 232.00         | Ni      | U2          |
| 279.48         | Mn      | U3          | 231.60         | Ni II   | V1          |
| 279.08         | Mg II   | V2          | 231.15         | Sb      | U1          |
| 278.02         | As      | U1          | 230.61         | In II   | V1          |
| 277.34         | Hf II   | V1          | 228.81         | As      | U5          |
| 276.78         | Tl      | U4          | 228.80         | Cd      | U2          |
| 272.44         | W       | U4          | 228.71         | Ni II   | V1          |
| 271.90         | Fe      | U5          | 228.62         | Co II   | V1          |
| 271.47         | Ta      | U1          | 228.23         | Os II   | V2          |
| 270.65         | Sn      | U4          | 227.66         | Bi      | U3          |
| 267.72         | Cr II   | V1          | 227.02         | Ni II   | V2          |
| 267.60         | Au      | U2          | 226.50         | Cd II   | V2          |
| 266.92         | Al II   | V1          | 226.45         | Ni II   | V3          |
| 265.95         | Pt      | U1          | 225.58         | Os II   | V1          |
| 265.12         | Ge      | U1          | 225.39         | Ni II   | V4          |
| 265.05         | Ba      | U2          | 224.70         | Cu II   | V3          |
| 264.75         | Ta      | U2          | 224.64         | Ag II   | V3          |
| 263.87         | Hf II   | V1          | 224.60         | Sn      | U1          |
| 263.71         | Os      | U1          | 224.27         | Ir II   | V1          |
| 260.57         | Mn II   | V3          | 223.06         | Bi      | U1          |
| 259.94         | Fe II   | V1          | 220.35         | Pb II   | V1          |
| 259.81         | Sb      | U2          | 219.87         | Ge II   | V2          |
| 259.37         | Mn      | U2          | 219.23         | Cu II   | V2          |
| 257.61         | Mn II   | V1          | 217.58         | Sb      | U2          |
| 256.37         | Mn II   | V2          | 217.00         | Pb II   | V1          |
| 255.33         | P       | U3          | 214.44         | Cd II   | V1          |
| 255.24         | Sc II   | V3          | 214.42         | Pt II   | V1          |
| 253.65         | Hg      | U1          | 214.27         | Te      | U1          |
| 253.57         | P       | U1          | 213.86         | Zn      | U1          |
| 252.85         | Si      | U2          | 213.62         | P       | U1          |
| 252.29         | Fe      | U3          | 213.60         | Cu II   | V1          |
| 251.61         | Si      | U3          | 212.68         | Ir II   | V1          |
| 250.69         | Si      | U4          | 209.48         | W II    | V2          |
| 250.20         | Zn II   | V4          | 209.43         | Ge II   | V1          |
| 249.77         | B       | U1          | 208.88         | Ir      | U1          |
| 249.68         | B       | U2          | 207.91         | W II    | V1          |
| 248.33         | Fe      | U3          | 207.48         | Se      | U4          |
| 247.86         | C       | U2          | 206.83         | Sb      | U1          |
| 245.65         | As      | U4          | 206.28         | Se      | U3          |
| 243.78         | Ag II   | V2          | 206.19         | Zn II   | V2          |
| 242.80         | Au      | U1          | 203.99         | Se      | U1          |
| 241.05         | Fe II   | V4          | 203.84         | Mo II   | V3          |
| 240.73         | Co      | U1          | 202.55         | Zn II   | V1          |
| 240.49         | Fe      | V3          | 202.03         | Mo II   | V2          |
| 240.27         | Ru      | V1          | 197.31         | Re II   | V1          |
| 240.06         | Ta II   | V1          | 197.20         | As      | U3          |

TABLE 7.19 Sensitive Lines of the Elements (Continued)

| Wavelength, nm | Element | Sensitivity | Wavelength, nm | Element | Sensitivity |
|----------------|---------|-------------|----------------|---------|-------------|
| 196.03         | Se      | U2          | 183.00         | I       | U2          |
| 194.23         | Hg II   | V1          | 182.59         | B II    | V2          |
| 193.76         | As      | U1          | 180.73         | S       | U1          |
| 193.09         | C       | U1          | 178.38         | I       | U1          |
| 190.86         | Tl II   | V1          | 178.28         | P       | U1          |
| 189.99         | Sn II   | V1          | 154.07         | Br II   | V4          |
| 189.04         | As      | U2          | 134.72         | Cl II   | V1          |

are steady-state techniques, are compared with the electrothermal or furnace technique which uses the entire sample and detects an absolute amount of the analyte element. To compare the several methods on the basis of concentration, the furnace detection limits assume a 20-μL sample.

Data for the several flame methods assume an acetylene–nitrous oxide flame residing on a 5- or 10-cm slot burner. The sample is nebulized into a spray chamber placed immediately ahead of the burner. Detection limits are quite dependent on instrument and operating variables, particularly the detector, the fuel and oxidant gases, the slit width, and the method used for background correction and data smoothing.

7.4.1 Some Common Spectroscopic Relationships

**7.4.1.1 Electromagnetic Radiation.** Electromagnetic radiation travels in straight lines in a uniform medium, has a velocity of 299 792 500 m · s<sup>-1</sup> in a vacuum, and possesses properties of both a wave motion and a particle (photon). *Wavelength* λ is the distance from crest to crest; *frequency* ν is the number of waves passing a fixed point in a unit length of time. Wavelength and frequency are related by the relation

$$c = \lambda \nu$$

where *c* is the velocity of light (in a vacuum). In any material medium the speed of propagation is smaller than this and is given by the product *nc*, where *n* is the refractive index of the medium.

Radiation is absorbed or emitted only in discrete packets called photons and quanta:

$$E = h\nu$$

where *E* is the energy of the quantum and *h* is Planck’s constant.

The relation between energy and mass is given by the *Einstein equation*:

$$\Delta E = \Delta mc^2$$

where Δ*E* is the energy release and Δ*m* is the loss of mass. Strictly, the mass of a particle depends on its velocity, but here the masses are equated to their rest masses (at zero velocity).

The *Wien displacement law* states that the wavelength of maximum emission, λ<sub>*m*</sub>, of a blackbody varies inversely with absolute temperature; the product λ<sub>*m*</sub>*T* remains constant. When λ<sub>*m*</sub> is expressed in micrometers, the law becomes

$$\lambda_m T = 2898$$

In terms of  $\sigma_m$ , the wavenumber of maximum emission:

$$\sigma_m = 3.48T$$

Another useful version is  $h\nu_m = 5kT$ , where  $k$  is the Boltzmann constant.

*Stefan's law* states that the total energy  $J$  radiated by a blackbody per unit time and area (power per unit area) varies as the fourth power of the absolute temperature:

$$J = aT^{-4}$$

where  $a$  is a constant whose value is  $5.67 \times 10^{-8} \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$ .

The relationship between the voltage of an X-ray tube (or other energy source), in volts, and the wavelength is given by the *Duane-Hunt equation*:

$$\lambda = \frac{hc}{eV} = \frac{12\,398}{V}$$

where the wavelength is expressed in angstrom units.

**7.4.1.2 Laws of Photometry.** The time rate at which energy is transported in a beam of radiant energy is denoted by the symbol  $P_0$  for the incident beam, and by  $P$  for the quantity remaining unabsorbed after passage through a sample or container. The ratio of radiant power transmitted by the sample to the radiant power incident on the sample is the *transmittance*  $T$ :

$$T = \frac{P}{P_0}$$

The logarithm (base 10) of the reciprocal of the transmittance is the *absorbance*  $A$ :

$$A = -\log T = \log \left( \frac{1}{T} \right)$$

When a beam of monochromatic light, previously rendered plane parallel, enters an absorbing medium at right angles to the plane-parallel surfaces of the medium, the rate of decrease in radiant power with the length of light path (cuvette interior)  $b$ , or with the concentration of absorbing material  $C$  (in grams per liter) will follow the exponential progression, often referred to as *Beer's law*:

$$T = 10^{-abC} \quad \text{or} \quad A = abC$$

where  $a$  is the absorptivity of the component of interest in the solution. When  $C$  is expressed in moles per liter,

$$T = 10^{-\epsilon bC} \quad \text{or} \quad A = \epsilon bC$$

where  $\epsilon$  is the molar absorptivity.

The total fluorescence (or phosphorescence) intensity is proportional to the quanta of light absorbed,  $P_0 - P$ , and to the efficiency  $\phi$ , which is the ratio of quanta absorbed to quanta emitted:

$$F = (P_0 - P)\phi = P_0\phi(1 - e^{-\epsilon bC})$$

When the terms  $\epsilon bC$  is not greater than 0.05 (or 0.01 in phosphorescence),

$$F = k\phi P_0 \epsilon bC$$

where the term  $k$  has been introduced to handle instrumental artifacts and the geometry factor because fluorescence (and phosphorescence) is emitted in all directions but is viewed only through a limited aperture.

The thickness of a transparent film or the path length of infrared absorption cells  $b$ , in centimeters, is given by

$$b = \frac{1}{2n_D} \left( \frac{n}{\bar{\nu}_1 - \bar{\nu}_2} \right)$$

where  $n$  is the number of fringes (peaks or troughs) between two wavenumbers  $\bar{\nu}_1$  and  $\bar{\nu}_2$ , and  $n_D$  is the refractive index of the sample material (unity for the air path of an empty cuvette). If measurements are made in wavelength, as micrometers, the expression is

$$b = \frac{1}{2n_D} \left( \frac{n\lambda_1\lambda_2}{\lambda_2 - \lambda_1} \right)$$

**7.4.1.3 Grating Equation.** The light incident on each groove is diffracted or spread out over a range of angles, and in certain directions reinforcement or constructive interference occurs, as stated in the grating formula:

$$m\lambda = b(\sin i \pm \sin r)$$

where  $b$  is the distance between adjacent grooves,  $i$  is the angle of incidence,  $r$  is the angle of reflection (both angles relative to the grating normal), and  $m$  is the order number. A positive sign applies where incoming and emergent beams are on the same side of the grating normal.

The *blaze wavelength* is that wavelength for which the angle of reflectance from the groove face and the angle of reflection (usually the angle of incidence) from the grating are identical.

The *Bragg equation*

$$m\lambda = 2d \sin \theta$$

states the condition for reinforcement of reflection from a crystal lattice, where  $d$  is the distance between each set of atomic planes and  $\theta$  is the angle of reflection.

**7.4.1.4 Ionization of Metals in a Plasma.** A loss in spectrochemical sensitivity results when a free metal atom is split into a positive ion and an electron:



The degree of ionization,  $\alpha_i$ , is defined as

$$\alpha_i = \frac{[M^+]}{[M^+] + [M]}$$

At equilibrium, when the ionization and recombination rates are balanced, the ionization constant  $K_i$  (in atm) is given by

$$K_i = \frac{[M^+][e^-]}{[M]} = \left( \frac{\alpha_i^2}{1 - \alpha_i^2} \right) p_{\Sigma M}$$

where  $p_{\Sigma M}$  (in atm) is the total atom concentration of metal in all forms in the plasma.

The ionization constant can be calculated from the *Saha equation*:

$$\log K_i = -5040 \frac{E_i}{T} + \frac{5}{2} \log T - 6.49 + \log \frac{g_{M^+} g_{e^-}}{g_M}$$

where  $E_i$  is the ionization potential of the metal in eV (Table 4.2),  $T$  is the absolute temperature of the plasma (in kelvins), and the  $g$  terms are the statistical weights of the ionized atom, the electron, and the neutral atom. For the alkali metals the final term is zero; for the alkaline earth metals, it is 0.6.

To suppress the ionization of a metal, another easily ionized metal (denoted a *deionizer* or *radiation buffer*) is added to the sample. To ensure that ionization is suppressed for the test element, the product  $(K_i)_{MP_M}$  of the deionizer must exceed the similar product for the test element one hundred-fold (for 1 percent residual ionization of the test element).

## 7.5 INFRARED SPECTROSCOPY

**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen

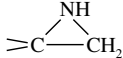
### Abbreviations Used in the Table

|                         |                                |
|-------------------------|--------------------------------|
| m, moderately strong    | var, of variable strength      |
| m-s, moderate to strong | w, weak                        |
| s, strong               | w-m, weak to moderately strong |

| Group                                                                                            | Band, $\text{cm}^{-1}$                                          | Remarks                                                                                                                                                                                                                           |
|--------------------------------------------------------------------------------------------------|-----------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Saturated C—H                                                                                    |                                                                 |                                                                                                                                                                                                                                   |
| $\begin{array}{c} \text{H} \\   \\ -\text{C}-\text{H} \\   \\ \text{H} \end{array}$              | 2975–2950 (s)<br>2885–2865 (w)<br><br>1450–1260 (m)             | Two or three bands usually; asymmetrical and symmetrical CH stretching, respectively. In presence of double bond adjacent to $\text{CH}_3$ group symmetrical band splits into two.<br>Sensitive to adjacent negative substituents |
| $\begin{array}{c} \text{H} \\   \\ -\text{C}- \\   \\ \text{H} \end{array} \quad \text{acyclic}$ | ca 2930 (s)<br>2870–2840 (w)<br><br>1480–1440 (m)<br>ca 720 (w) | Frequency increased in strained systems. Symmetrical band splits into two bands when double bond adjacent.<br>Scissoring mode<br>Rocking mode                                                                                     |
| Alkane residues attached to carbon                                                               |                                                                 |                                                                                                                                                                                                                                   |
| Cyclopropane                                                                                     | ca 3050 (w)<br>540–500<br>470–460 (s)                           | CH stretching<br><br>Aliphatic cyclopropanes                                                                                                                                                                                      |
| Cyclobutanes                                                                                     | 580–490 (s)                                                     | Alkyl derivatives: 550–530 $\text{cm}^{-1}$                                                                                                                                                                                       |
| Cyclopentanes                                                                                    | 595–490 (s)                                                     | Alkyl derivatives: 585–530 $\text{cm}^{-1}$                                                                                                                                                                                       |



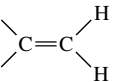
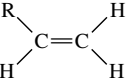
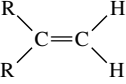
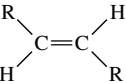
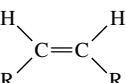
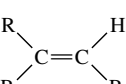
**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen (*Continued*)

| Group                                                                                                            | Band, $\text{cm}^{-1}$                                           | Remarks                                                                                               |
|------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Alkane residues attached to carbon ( <i>continued</i> )                                                          |                                                                  |                                                                                                       |
| $\text{>C}(\text{CH}_3)_2$                                                                                       | ca 1380 (m)<br>1175–1165 (m)<br>1150–1130 (m)                    | A roughly symmetrical doublet<br>If no H on central carbon, then one band at ca $1190\text{ cm}^{-1}$ |
| $\text{—C}(\text{CH}_3)_3$                                                                                       | 1395–1385 (m)<br>1365 (s)                                        | Split into two bands                                                                                  |
| Aryl- $\text{CH}_3$<br>Aryl- $\text{C}_2\text{H}_5$<br>Aryl- $\text{C}_3\text{H}_7$ (or $\text{C}_4\text{H}_9$ ) | 390–260 (m)<br>565–540 (m-s)<br>585–565 (m)                      | Two bands                                                                                             |
| $\text{—}(\text{CH}_2)_n\text{—}$<br>$n = 1$<br>$n = 2$<br>$n = 3$<br>$n \geq 4$                                 | 785–770 (w-m)<br>745–735 (w-m)<br>735–725 (w-m)<br>725–720 (w-m) | Rocking vibrations                                                                                    |
| Alkane residues attached to miscellaneous atoms                                                                  |                                                                  |                                                                                                       |
| Epoxide C—H<br>                  | ca 3050 (m-s)<br>ca 3050 (m-s)                                   |                                                                                                       |
| $\text{—CH}_2\text{—halogen}$                                                                                    | ca 3050 (m-s)<br>1435–1385 (m)<br>1300–1240 (s)                  | Halogens except fluorine                                                                              |
| $\text{—CHO}$                                                                                                    | 2900–2800 (w)<br>2775–2700 (w)<br>1420–1370 (m)                  |                                                                                                       |
| $\text{—CO—CH}_3$                                                                                                | 3100–2900 (w)<br>1450–1400 (s)<br>1360–1355 (s)                  |                                                                                                       |
| $\text{—O—CH}_3$ ethers                                                                                          | 2835–2810 (s)<br>1470–1430 (m-s)<br>ca 1030 (w-m)                | Two bands                                                                                             |
| $\text{—O—C}(\text{CH}_3)_3$                                                                                     | 1200–1155 (s)                                                    |                                                                                                       |
| $\text{—O—CH}_2\text{—O—}$                                                                                       | 2790–2770 (m)                                                    |                                                                                                       |
| $\text{—O—CH}_2\text{—}$ esters                                                                                  | 1475–1460 (m-s)<br>1470–1435 (m-s)                               | Acyclic esters. Frequency increased ca $30\text{ cm}^{-1}$ for cyclic and small ring systems.         |

**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen (*Continued*)

| Group                                                                                                                                                                                                                                                        | Band, cm <sup>-1</sup>                                                                                                                                                                                   | Remarks                                                                                          |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------|
| Alkane residues attached to miscellaneous atoms ( <i>continued</i> )                                                                                                                                                                                         |                                                                                                                                                                                                          |                                                                                                  |
| —O—CO—CH <sub>3</sub>                                                                                                                                                                                                                                        | 1450–1400 (s)<br>1385–1365 (s)<br>1360–1355 (s)                                                                                                                                                          | Acetate esters<br>The high intensity of these bands often dominates this region of the spectrum. |
| —CH <sub>2</sub> — $\overset{\textstyle  }{\text{C}}=\text{C}\leq$                                                                                                                                                                                           | 1445–1430 (m)                                                                                                                                                                                            |                                                                                                  |
| —CH <sub>2</sub> —SO <sub>2</sub> —                                                                                                                                                                                                                          | ca 1250 (m)                                                                                                                                                                                              |                                                                                                  |
| P—CH <sub>3</sub><br>Se—CH <sub>3</sub><br>B—CH <sub>3</sub><br>Si—CH <sub>3</sub><br>Sn—CH <sub>3</sub><br>Pb—CH <sub>3</sub><br>As—CH <sub>3</sub><br>Ge—CH <sub>3</sub><br>Sb—CH <sub>3</sub><br>Bi—CH <sub>3</sub><br>—CH <sub>2</sub> —(Cd, Hg, Zn, Sn) | 1320–1280 (s)<br>ca 1280 (m)<br>1460–1405 (m)<br>1320–1280 (m)<br>1265–1250 (m–s)<br>1200–1180 (m)<br>1170–1155 (m)<br>1265–1240 (m)<br>1240–1230 (m)<br>1215–1195 (m)<br>1165–1145 (m)<br>1430–1415 (m) |                                                                                                  |
| N—CH <sub>3</sub> and N—CH <sub>2</sub> —<br>N—CH <sub>2</sub> —CH <sub>2</sub> —N<br>N—CH <sub>3</sub><br>Amine · HCl<br>Amino acid · HCl<br>Amides<br>N—CH <sub>2</sub> — amides                                                                           | 2820–2780 (s)<br>1440–1390 (m)<br>1480–1450 (s)<br>1475–1395 (m)<br>1490–1480 (m)<br>1420–1405 (s)<br>ca 1440 (m)                                                                                        | Ethylenediamine complexes<br>Ethylenediamine complexes                                           |
| S—CH <sub>3</sub>                                                                                                                                                                                                                                            | 2990–2955 (m–s)<br>2900–2865 (m–s)<br>1440–1415 (m)<br>1325–1290 (m)<br>1030–960 (m)<br>710–685 (w–m)                                                                                                    |                                                                                                  |
| S—CH <sub>2</sub> —                                                                                                                                                                                                                                          | 2950–2930 (m)<br>2880–2845 (m)<br>1440–1415 (m)<br>1270–1220 (s)                                                                                                                                         |                                                                                                  |
| —C≡CH                                                                                                                                                                                                                                                        | ca 3300 (s)<br>700–600                                                                                                                                                                                   | Sharp<br>Bending                                                                                 |
| $\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array} \text{H}$                                                                                                                                                                            | 3040–3010 (m)                                                                                                                                                                                            |                                                                                                  |

**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen (*Continued*)

| Group                                                                                                                                                                                                                                                   | Band, $\text{cm}^{-1}$                                                                                             | Remarks                                                                                                         |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|
| Alkane residues attached to miscellaneous atoms ( <i>continued</i> )                                                                                                                                                                                    |                                                                                                                    |                                                                                                                 |
|                                                                                                                                                                         | 3095–3075 (m)<br>2985–2970 (m)                                                                                     | CH stretching sometimes obscured by much stronger bands of saturated CH groups                                  |
|                                                                                                                                                                         | 995–980 (s)<br>940–900 (s)<br>ca 635 (s)<br>485–445 (m–s)                                                          |                                                                                                                 |
|                                                                                                                                                                         | 895–885 (s)<br>560–530 (s)<br>470–435 (m)                                                                          |                                                                                                                 |
|                                                                                                                                                                         | 980–955 (s)<br>455–370 (m–s)                                                                                       |                                                                                                                 |
|                                                                                                                                                                         | 730–655 (m)<br>670–455 (s)                                                                                         |                                                                                                                 |
|                                                                                                                                                                         | 850–790 (m)<br>570–515 (s)<br>525–470 (s)                                                                          |                                                                                                                 |
| $-\text{O}-\text{CH}=\text{CH}_2$                                                                                                                                                                                                                       | 965–960 (s)<br>945–940 (m)<br>820–810 (s)                                                                          |                                                                                                                 |
| $-\text{S}-\text{CH}=\text{CH}_2$                                                                                                                                                                                                                       | ca 965 (s)<br>ca 860 (s)                                                                                           |                                                                                                                 |
| $-\text{CO}-\text{CH}=\text{CH}_2$<br>$-\text{CO}-\text{OCH}=\text{CH}_2$<br>$-\text{CO}-\text{C}=\text{CH}_2$<br>$-\text{CO}-\text{OC}=\text{CH}_2$<br>$-\text{O}-\text{CH}=\text{CH}-$ <i>trans</i><br>$-\text{CO}-\text{CH}=\text{CH}-$ <i>trans</i> | 995–980 (s)<br>965–955 (m)<br>950–935 (s)<br>870–850 (s)<br>ca 930 (s)<br>880–865 (s)<br>940–920 (s)<br>ca 990 (s) |                                                                                                                 |
| Hydroxyl group O—H compounds                                                                                                                                                                                                                            |                                                                                                                    |                                                                                                                 |
| Primary aliphatic alcohols                                                                                                                                                                                                                              | 3640–3630 (s)<br><br>1350–1260 (s)<br>1085–1030 (s)                                                                | Only in very dilute solutions in nonpolar solvents<br>OH bending<br>Also broad band at 700–600 $\text{cm}^{-1}$ |

**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen (*Continued*)

| Group                                             | Band, $\text{cm}^{-1}$ | Remarks                                                                                                                                   |
|---------------------------------------------------|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Hydroxyl group O—H compounds ( <i>continued</i> ) |                        |                                                                                                                                           |
| Secondary aliphatic alcohols                      | 3625–3620 (s)          | See comments under primary aliphatic alcohols                                                                                             |
|                                                   | 1350–1260 (s)          |                                                                                                                                           |
|                                                   | 1125–1085 (s)          | Also for $\alpha$ -unsaturated and cyclic tertiary aliphatic alcohols                                                                     |
| Tertiary aliphatic alcohols                       | 3620–3610 (s)          | See comments under primary aliphatic alcohols                                                                                             |
|                                                   | 1410–1310 (s)          |                                                                                                                                           |
|                                                   | 1205–1125 (s)          |                                                                                                                                           |
| Aryl—OH                                           | ca 3610 (s)            | See comments under primary aliphatic alcohols                                                                                             |
|                                                   | 1410–1310 (s)          |                                                                                                                                           |
|                                                   | 1260–1180 (s)          | Also for unsaturated secondary aliphatic alcohols                                                                                         |
|                                                   | 1085–1030 (s)          |                                                                                                                                           |
| Carboxylic acids                                  | 3300–2500 (w–m)        | Broad                                                                                                                                     |
|                                                   | 995–915 (s)            | Broad diffuse band                                                                                                                        |
| Enol form of $\beta$ -diketones                   | 2700–2500 (var)        | Broad                                                                                                                                     |
| Free oximes                                       | 3600–3570 (w–m)        | Shoulder                                                                                                                                  |
| Free hydroperoxides                               | 3560–3530 (m)          |                                                                                                                                           |
| Peroxy acids                                      | ca 3280 (m)            |                                                                                                                                           |
| Phosphorus acids                                  | 2700–2560 (m)          | Broad                                                                                                                                     |
| Water in solution                                 | 3710                   | When solution is damp                                                                                                                     |
| Intermolecular H bond                             |                        |                                                                                                                                           |
| Dimeric                                           | 3600–3500              | Rather sharp. Absorptions arising from H bond with polar solvents also appear in this region.                                             |
| Polymeric                                         | 3400–3200 (s)          | Broad                                                                                                                                     |
| Intramolecular H bond                             |                        |                                                                                                                                           |
| Polyvalent alcohols                               | 3600–3500 (s)          | Sharper than dimeric band above                                                                                                           |
| Chelation                                         | 3200–2500              | Broad and occasionally weak; the lower the frequency, the stronger the intramolecular bond                                                |
| Water of crystallation<br>(solid state spectra)   | 3600–3100 (w)          | Usually a weak band at 1640–1615 $\text{cm}^{-1}$ also. Water in trace amounts in KBr disks shows a broad band at 3450 $\text{cm}^{-1}$ . |

**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen (*Continued*)

| Group                                                          | Band, $\text{cm}^{-1}$ | Remarks                                                                                         |
|----------------------------------------------------------------|------------------------|-------------------------------------------------------------------------------------------------|
| Amine, imine, ammonium, and amide N—H                          |                        |                                                                                                 |
| Primary amines                                                 | 3550–3300 (m)          | Two bands in this range                                                                         |
| Aliphatic                                                      | 1650–1560 (m)          |                                                                                                 |
|                                                                | 1090–1020 (w–m)        | With $\alpha$ -carbon branching at $795\text{ cm}^{-1}$ and strong                              |
|                                                                | 850–810 (w–m)          |                                                                                                 |
|                                                                | 495–445 (m–s)          | Broad                                                                                           |
|                                                                | ca 290 (s)             | Broad                                                                                           |
| Aromatic                                                       | 1350–1260 (s)          | Also for secondary aryl amines                                                                  |
|                                                                | 445–345                |                                                                                                 |
| Amino acids                                                    | 3100–3030 (m)          | Values for solid states; broad bands also (but not always) near $2500$ and $200\text{ cm}^{-1}$ |
|                                                                | 2800–2400 (m)          | Number of sharp bands; dilute solution                                                          |
|                                                                | 1625–1560 (m)          |                                                                                                 |
|                                                                | 1550–1550 (m)          |                                                                                                 |
| Amino salts                                                    | 3550–3100 (m)          | Values for solid state                                                                          |
|                                                                | ca 3380                | Dilute solutions                                                                                |
|                                                                | ca 3280                |                                                                                                 |
| Secondary amines                                               | 3550–3400 (w)          | Only one band, whereas primary amines show two bands                                            |
|                                                                | 1580–1490 (w)          | Often too weak to be noticed                                                                    |
|                                                                | 1190–1170 (m)          |                                                                                                 |
|                                                                | 1145–1130 (m)          |                                                                                                 |
|                                                                | 455–405 (w–m)          |                                                                                                 |
| Salts                                                          | ca 2500                | Sharp; broad values for solid state                                                             |
|                                                                | ca 2400                | Sharp; broad values for solid state                                                             |
|                                                                | 1620–1560 (m–s)        |                                                                                                 |
| Tertiary amines<br>$\text{R}_1\text{R}_2\text{R}_3\text{NH}^+$ | 2700–2250              | Group of relatively sharp bands; broad bands in solid state                                     |
| Ammonium ion                                                   | 3300–3030 (s)          | Group of bands                                                                                  |
|                                                                | 1430–1390 (s)          |                                                                                                 |
| Imines $=\text{N}=\text{H}$                                    | 3350–3310 (w)          | Aliphatic                                                                                       |
|                                                                | 3490 (s)               | Aryl                                                                                            |
|                                                                | 3490 (s)               | Pyrroles, indoles; band sharp                                                                   |
| Imine salts                                                    | 2700–2330 (m–s)        | Dilute solutions                                                                                |
|                                                                | 2200–1800 (m)          | One or more bands; useful to distinguish from protonated tertiary amines                        |
| Primary amide $-\text{CONH}_2$                                 | ca 3500 (m)            | Lowered ca $150\text{ cm}^{-1}$ in the solid state                                              |
|                                                                | ca 3400 (m)            | and on H bonding; often several bands $3200\text{--}3050\text{ cm}^{-1}$                        |
| Secondary amide<br>$-\text{CONH}-$                             | 3460–3400 (m)          | Two bands; lowered on H bonding and in solid state. Only one band with lactams                  |
|                                                                | 3100–3070 (w)          | Extra band with bonded and solid-state samples                                                  |

**TABLE 7.20** Absorption Frequencies of Single Bonds to Hydrogen (*Continued*)

| Group                                                                                                    | Band, $\text{cm}^{-1}$                       | Remarks                                                                               |
|----------------------------------------------------------------------------------------------------------|----------------------------------------------|---------------------------------------------------------------------------------------|
| Miscellaneous R—H                                                                                        |                                              |                                                                                       |
| —S—H                                                                                                     | 2600–2550 (w)                                | Weaker than OH and less affected by H bonding                                         |
| P—H                                                                                                      | 2440–2350 (m)                                | Sharp                                                                                 |
| $\begin{array}{c} \text{O} \\ \parallel \\ \text{P} \\ \diagup \quad \diagdown \\ \text{OH} \end{array}$ | 2700–2560 (m)                                | Associated OH                                                                         |
| R—D                                                                                                      | 100/137 times the corresponding RH frequency | Useful when assigning RH bands; deuteration leads to a known shift to lower frequency |

**TABLE 7.21** Absorption Frequencies of Triple Bonds*Abbreviations Used in the Table*

|                         |                                |
|-------------------------|--------------------------------|
| m, moderately strong    | var, of variable strength      |
| m–s, moderate to strong | w–m, weak to moderately strong |
| s, strong               |                                |

| Group                                   | Band, $\text{cm}^{-1}$                                           | Remarks                                                                                                                                                                                                                                                                                                                                                      |
|-----------------------------------------|------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Alkynes                                 |                                                                  |                                                                                                                                                                                                                                                                                                                                                              |
| Terminal                                | 3300 (s)<br>2140–2100 (w–m)*<br>1375–1225 (w–m)<br>695–575 (m–s) | CH stretching<br>C≡C stretching                                                                                                                                                                                                                                                                                                                              |
| Nonterminal                             | ca 630 (s)<br>2260–2150 (var)*                                   | Two bands if molecule has axial symmetry<br>Alkyl monosubstituted<br>Symmetrical or nearly symmetrical substitution makes the C≡C stretching frequency inactive. When more than one C≡C linkage is present, and sometimes when there is only one, there are frequently more absorption bands in this region than there are triple bonds to account for them. |
| $\text{R}_1\text{—C}\equiv\text{C—R}_2$ | 540–465 (m)                                                      | The longer the chain, the lower the frequency                                                                                                                                                                                                                                                                                                                |
| Aryl—C≡C—                               | ca 550 (m)<br>ca 350 (var)                                       |                                                                                                                                                                                                                                                                                                                                                              |
| —C≡C—halogen (Cl, Br, I)                | 185–160 (var)                                                    |                                                                                                                                                                                                                                                                                                                                                              |

\* Conjugation with olefinic or acetylenic groups lowers the frequency and raises the intensity. Conjugation with carbonyl groups usually has little effect on the position of absorption.

TABLE 7.21 Absorption Frequencies of Triple Bonds (Continued)

| Group                                                     | Band, cm <sup>-1</sup>                           | Remarks                                                                                          |
|-----------------------------------------------------------|--------------------------------------------------|--------------------------------------------------------------------------------------------------|
| Nitriles —C≡N                                             | 2260–2200 (var)                                  | Stronger and toward the lower end of the range when conjugated; occasionally very weak or absent |
| Aliphatic                                                 | 580–555 (m–s)                                    |                                                                                                  |
|                                                           | 560–525 (m–s)                                    |                                                                                                  |
|                                                           | 390–350 (s)                                      |                                                                                                  |
| Aromatic                                                  | 580–540 (s)                                      |                                                                                                  |
|                                                           | 430–380 (m)                                      |                                                                                                  |
| Isonitriles R—N <sup>+</sup> ≡C <sup>−</sup><br>or R—N=C: | 2175–2150 (s)<br>2150–2115 (s)<br>1595           | Very sensitive to changes in substituents<br>Not found for nitriles                              |
| Cyanamides<br>>N—C≡N ⇌ >N <sup>+</sup> —C= N <sup>−</sup> | 2225–2210 (s)                                    |                                                                                                  |
| Thiocyanates<br>R—S—C≡N                                   | 2175–2140 (s)<br><br>404–400 (s)<br>ca 600 (m–s) | Aryl thiocyanates at the upper end of the range, alkyl at the lower end<br>Aliphatic derivatives |
| Nitrile N-oxides<br>—C≡N→O                                | 2305–2285 (s)<br>1395–1365 (s)                   | Aryl derivatives                                                                                 |
| Diazonium salts<br>R—N≡N                                  | 2300–2230 (m–s)                                  |                                                                                                  |
| Selenocyanates<br>R—Se—C≡N                                | ca 2160 (m–s)<br>545–520<br>ca 390<br>ca 350     |                                                                                                  |

**TABLE 7.22** Absorption Frequencies of Cumulated Double Bonds*Abbreviations Used in the Table*

m–s, moderate to strong

vs, very strong

s, strong

w, weak

| Group                                                                                            | Band, $\text{cm}^{-1}$                                            | Remarks                                                                                                |
|--------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
| Carbon dioxide<br>$\text{O}=\text{C}=\text{O}$                                                   | 2349 (s)                                                          | Appears in many spectra as a result of inequalities in path length                                     |
| Isocyanates<br>$-\text{N}=\text{C}=\text{O}$                                                     | 2275–2250 (vs)                                                    | Position unaffected by conjugation                                                                     |
| Isoselenocyanates<br>$-\text{N}=\text{C}=\text{Se}$                                              | 2200–2000 (s)<br>675–605                                          | Broad; usually two bands                                                                               |
| Azides<br>$-\text{N}_3$ or $-\text{N}=\text{N}^+=\text{N}^-$                                     | 2140–2030 (s)<br>1340–1180 (w)                                    | Not observed for ionic azides                                                                          |
| $-\text{N}=\text{C}=\text{N}-$                                                                   | 2155–2130 (s)                                                     | Split into unsymmetrical doublet by conjugation with aryl groups:<br>2145–2125 (vs) and 2115–2105 (vs) |
| Isothiocyanates<br>$-\text{N}=\text{C}=\text{S}$                                                 | 2140–1990 (vs)<br>649–600 (m–s)<br>565–510 (m–s)<br>470–440 (m–s) | Broad; usually a doublet                                                                               |
| Ketenes<br>$>\text{C}=\text{C}=\text{O}$                                                         | ca 2150 (s)                                                       |                                                                                                        |
| Ketenimines<br>$\text{C}=\text{C}=\text{N}-$                                                     | 2050–2000 (s)                                                     |                                                                                                        |
| Allenes<br>$>\text{C}=\text{C}=\text{C}<$                                                        | 2000–1915 (m–s)                                                   | Two bands when terminal allene or when bonded to electron-attracting groups                            |
| Thionylamines<br>$-\text{N}=\text{S}=\text{O}$                                                   | 1300–1230 (s)<br>1180–1110 (s)                                    |                                                                                                        |
| Diazoalkanes<br>$\text{R}_2\text{C}=\text{N}^+=\text{N}^-$<br>$-\text{CH}=\text{N}^+=\text{N}^-$ | 2030–2000 (s)<br>2050–2035 (s)                                    |                                                                                                        |
| Diazoketones<br>$-\text{CO}-\text{CH}=\text{N}^+=\text{N}^-$                                     | 2100–2080<br>2075–2050                                            | Monosubstituted<br>Disubstituted                                                                       |



**TABLE 7.23** Absorption Frequencies of Carbonyl Bands*All bands quoted are strong.*

| Groups                                                                 | Band, $\text{cm}^{-1}$                                | Remarks                                                                                                                                                                                        |
|------------------------------------------------------------------------|-------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Acid anhydrides</b><br>—CO—O—CO—                                    |                                                       |                                                                                                                                                                                                |
| Saturated                                                              | 1850–1800<br>1790–1740                                | Two bands usually separated by about 60 $\text{cm}^{-1}$ . The higher-frequency band is more intense in acyclic anhydrides, and the lower-frequency band is more intense in cyclic anhydrides. |
| Aryl and $\alpha,\beta$ -unsaturated                                   | 1830–1780<br>1790–1710                                |                                                                                                                                                                                                |
| Saturated five-ring                                                    | 1870–1820<br>1800–1750                                |                                                                                                                                                                                                |
| All classes                                                            | 1300–1050                                             |                                                                                                                                                                                                |
| <b>Acid chlorides</b> —COCl                                            |                                                       |                                                                                                                                                                                                |
| Saturated                                                              | 1815–1790                                             | Acid fluorides higher, bromides and iodides lower                                                                                                                                              |
| Aryl and $\alpha,\beta$ -unsaturated                                   | 1790–1750                                             |                                                                                                                                                                                                |
| <b>Acid peroxide</b><br>CO—O—O—CO—                                     |                                                       |                                                                                                                                                                                                |
| Saturated                                                              | 1820–1810<br>1800–1780                                |                                                                                                                                                                                                |
| Aryl and $\alpha,\beta$ -unsaturated                                   | 1805–1780<br>1785–1755                                |                                                                                                                                                                                                |
| <b>Esters and lactones</b><br>—CO—O—                                   |                                                       |                                                                                                                                                                                                |
| Saturated                                                              | 1750–1735                                             |                                                                                                                                                                                                |
| Aryl and $\alpha,\beta$ -unsaturated                                   | 1730–1715                                             |                                                                                                                                                                                                |
| Aryl and vinyl esters<br>C=C—O—CO—alkyl                                | 1800–1750                                             | The C=C stretching band also shifts to higher frequency.                                                                                                                                       |
| Esters with electronegative $\alpha$ substituents; e.g.,<br>>CCl—CO—O— | 1770–1745                                             |                                                                                                                                                                                                |
| $\alpha$ -Keto esters                                                  | 1755–1740                                             |                                                                                                                                                                                                |
| Six-ring and larger lactones                                           | Similar values to the corresponding open-chain esters |                                                                                                                                                                                                |
| Five-ring lactone                                                      | 1780–1760                                             |                                                                                                                                                                                                |
| $\alpha,\beta$ -Unsaturated five-ring lactone                          | 1770–1740                                             | When $\alpha$ -CH is present, there are two bands, the relative intensity depending on the solvent.                                                                                            |
| $\beta,\gamma$ -Unsaturated five-ring lactone, vinyl ester type        | ca 1800                                               |                                                                                                                                                                                                |
| Four-ring lactone                                                      | ca 1820                                               |                                                                                                                                                                                                |
| $\beta$ -Keto ester in H bonding enol form                             | ca 1650                                               | Keto from normal; chelate-type H bond causes shift to lower frequency than the normal ester. The C=C band is strong and is usually near 1630 $\text{cm}^{-1}$ .                                |
| All classes                                                            | 1300–1050                                             |                                                                                                                                                                                                |
|                                                                        |                                                       | Usually two strong bands due to CO stretching                                                                                                                                                  |

**TABLE 7.23** Absorption Frequencies of Carbonyl Bands (*Continued*)

| Groups                                                                                                                                                                                                       | Band, $\text{cm}^{-1}$                                 | Remarks                                                                                                                                                 |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Aldehydes —CHO</b>                                                                                                                                                                                        |                                                        |                                                                                                                                                         |
| (See also Table 7.49 for C—H.) All values given below are lowered in liquid-film or solid-state spectra by about 10–20 $\text{cm}^{-1}$ . Vapor-phase spectra have values raised about 20 $\text{cm}^{-1}$ . |                                                        |                                                                                                                                                         |
| Saturated                                                                                                                                                                                                    | 1740–1720                                              |                                                                                                                                                         |
| Aryl                                                                                                                                                                                                         | 1715–1695                                              | <i>o</i> -Hydroxy or amino groups shift this value to 1655–1625 $\text{cm}^{-1}$ because of intramolecular H bonding.                                   |
| $\alpha,\beta$ -Unsaturated                                                                                                                                                                                  | 1705–1680                                              |                                                                                                                                                         |
| $\alpha,\beta,\gamma,\delta$ -Unsaturated                                                                                                                                                                    | 1680–1660                                              |                                                                                                                                                         |
| $\beta$ -Ketoaldehyde in enol form                                                                                                                                                                           | 1670–1645                                              | Lowering caused by chelate-type H bonding                                                                                                               |
| <b>Ketones &gt;C=O</b>                                                                                                                                                                                       |                                                        |                                                                                                                                                         |
| All values given below are lowered in liquid-film or solid-state spectra by about 10–20 $\text{cm}^{-1}$ . Vapor-phase spectra have values raised about 20 $\text{cm}^{-1}$ .                                |                                                        |                                                                                                                                                         |
| Saturated                                                                                                                                                                                                    | 1725–1705                                              |                                                                                                                                                         |
| Aryl                                                                                                                                                                                                         | 1700–1680                                              |                                                                                                                                                         |
| $\alpha,\beta$ -Unsaturated                                                                                                                                                                                  | 1685–1665                                              |                                                                                                                                                         |
| $\alpha,\beta,\alpha',\beta'$ -Unsaturated and diaryl                                                                                                                                                        | 1670–1660                                              |                                                                                                                                                         |
| Cyclopropyl                                                                                                                                                                                                  | 1705–1685                                              |                                                                                                                                                         |
| Six-ring ketones and larger                                                                                                                                                                                  | Similar values to the corresponding open-chain ketones |                                                                                                                                                         |
| Five-ring ketones                                                                                                                                                                                            | 1750–1740                                              | $\alpha,\beta$ Unsaturation, $\alpha,\beta,\alpha',\beta'$ unsaturation, etc., have a similar effect on these values as on those of open-chain ketones. |
| Four-ring ketones                                                                                                                                                                                            | ca 1780                                                |                                                                                                                                                         |
| $\alpha$ -Halo ketones                                                                                                                                                                                       | 1745–1725                                              | Affected by conformation; highest values are obtained when both halogens are in the same plane as the C=O.                                              |
| $\alpha,\alpha'$ -Dihalo ketones                                                                                                                                                                             | 1765–1745                                              |                                                                                                                                                         |
| 1,2-Diketones, <i>syn-trans</i> -open chains                                                                                                                                                                 | 1730–1710                                              | Antisymmetrical stretching frequency of both C=O's. The symmetrical stretching is inactive in the infrared but active in the Raman.                     |
| <i>syn-cis</i> -1,2-Diketones, six-ring                                                                                                                                                                      | 1760 and 1730                                          |                                                                                                                                                         |
| <i>syn-cis</i> -1,2-Diketones, five-ring                                                                                                                                                                     | 1775 and 1760                                          |                                                                                                                                                         |

**TABLE 7.23** Absorption Frequencies of Carbonyl Bands (*Continued*)

| Groups                                                                                                      | Band, $\text{cm}^{-1}$ | Remarks                                                                                                                                                                                                                                                                                        |
|-------------------------------------------------------------------------------------------------------------|------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Ketones</b> $\text{>C=O}$ ( <i>continued</i> )<br><i>o</i> -Amino-aryl or <i>o</i> -hydroxy-aryl ketones | 1655–1635              | Low because of intramolecular H bonding. Other substituents and steric hindrance affect the position of the band.                                                                                                                                                                              |
| Quinones                                                                                                    | 1690–1660              | C=C band is strong and is usually near $1600\text{ cm}^{-1}$ .                                                                                                                                                                                                                                 |
| Extended quinones                                                                                           | 1655–1635              |                                                                                                                                                                                                                                                                                                |
| Tropone                                                                                                     | 1650                   | Near $1600\text{ cm}^{-1}$ when lowered by H bonding as in tropolones                                                                                                                                                                                                                          |
| <b>Carboxylic acids</b> $\text{—CO}_2\text{H}$<br>All types                                                 | 3000–2500              | OH stretching; a characteristic group of small bands due to combination bands                                                                                                                                                                                                                  |
| Saturated                                                                                                   | 1725–1700              | The monomer is near $1760\text{ cm}^{-1}$ , but is rarely observed. Occasionally both bands, the free monomer, and the H-bonded dimer can be seen in solution spectra. Ether solvents give one band near $1730\text{ cm}^{-1}$ .                                                               |
| $\alpha,\beta$ -Unsaturated                                                                                 | 1715–1690              |                                                                                                                                                                                                                                                                                                |
| Aryl                                                                                                        | 1700–1680              |                                                                                                                                                                                                                                                                                                |
| $\alpha$ -Halo-                                                                                             | 1740–1720              |                                                                                                                                                                                                                                                                                                |
| <b>Carboxylate ions</b> $\text{—CO}_2^-$<br>Most types                                                      | 1610–1550<br>1420–1300 | Antisymmetrical and symmetrical stretching, respectively                                                                                                                                                                                                                                       |
| <b>Amides</b> $\text{—CO—N<}$<br>(See also Table 7.49 for NH stretching and bending.)                       |                        |                                                                                                                                                                                                                                                                                                |
| Primary $\text{—CONH}_2$                                                                                    |                        |                                                                                                                                                                                                                                                                                                |
| In solution                                                                                                 | ca 1690                | Amide I; C=O stretching                                                                                                                                                                                                                                                                        |
| Solid state                                                                                                 | ca 1650                |                                                                                                                                                                                                                                                                                                |
| In solution                                                                                                 | ca 1600                | Amide II; mostly NH bending                                                                                                                                                                                                                                                                    |
| Solid state                                                                                                 | ca 1640                | Amide I is generally more intense than amide II. (In the solid state, amides I and II may overlap.)                                                                                                                                                                                            |
| Secondary $\text{—CONH—}$                                                                                   |                        |                                                                                                                                                                                                                                                                                                |
| In solution                                                                                                 | 1700–1670              | Amide I                                                                                                                                                                                                                                                                                        |
| Solid state                                                                                                 | 1680–1630              |                                                                                                                                                                                                                                                                                                |
| In solution                                                                                                 | 1550–1510              | Amide II; found in open-chain amides only                                                                                                                                                                                                                                                      |
| Solid state                                                                                                 | 1570–1515              | Amide I is generally more intense than amide II.                                                                                                                                                                                                                                               |
| Tertiary                                                                                                    | 1670–1630              | Since H bonding is absent, solid and solution spectra are much the same.                                                                                                                                                                                                                       |
| Lactams                                                                                                     |                        |                                                                                                                                                                                                                                                                                                |
| Six-ring and larger rings                                                                                   | ca 1670                |                                                                                                                                                                                                                                                                                                |
| Five-ring                                                                                                   | ca 1700                | Shifted to higher frequency when the N atom is in a bridged system                                                                                                                                                                                                                             |
| Four-ring                                                                                                   | ca 1745                | Shifted $+15\text{ cm}^{-1}$ by the additional double bond                                                                                                                                                                                                                                     |
| $\text{R—CO—N—C}\equiv\text{C}$                                                                             |                        | Shifted by up to $+15\text{ cm}^{-1}$ by the additional double bond. This is an unusual effect by $\alpha,\beta$ unsaturation. It is said to be due to the inductive effect of the C=C on the well-conjugated CO—N system, the usual conjugation effect being less important in such a system. |
| $\text{C}\equiv\text{C—CO—N}$                                                                               |                        |                                                                                                                                                                                                                                                                                                |

**TABLE 7.23** Absorption Frequencies of Carbonyl Bands (*Continued*)

| Groups                                  | Band, $\text{cm}^{-1}$ | Remarks                                                                               |
|-----------------------------------------|------------------------|---------------------------------------------------------------------------------------|
| <b>Imides</b> —CO—N—CO—                 |                        |                                                                                       |
| Cyclic six-ring                         | ca 1710 and<br>ca 1700 | Shift of $+15 \text{ cm}^{-1}$ with $\alpha,\beta$ unsaturation                       |
| Cyclic five-ring                        | ca 1770 and<br>ca 1700 |                                                                                       |
| <b>Ureas</b> N—CO—N                     |                        |                                                                                       |
| RNHCONHR                                | ca 1660                |                                                                                       |
| Six-ring                                | ca 1640                |                                                                                       |
| Five-ring                               | ca 1720                |                                                                                       |
| <b>Urethanes</b> R—O—CO—N               | 1740–1690              | Also shows amide II band when nonsubstituted on N                                     |
| <b>Thioesters and Acids</b><br>RCO—S—R' |                        |                                                                                       |
| RCOSH                                   | ca 1720                | $\alpha,\beta$ -Unsaturated or aryl acid or ester shifted about $-25 \text{ cm}^{-1}$ |
| RCOS—alkyl                              | ca 1690                |                                                                                       |
| RCOS—aryl                               | ca 1710                |                                                                                       |

### 7.5.1 Intensities of Carbonyl Bands

Acids generally absorb more strongly than esters, and esters more strongly than ketones or aldehydes. Amide absorption is usually similar in intensity to that of ketones but is subject to much greater variations.

### 7.5.2 Position of Carbonyl Absorption

The general trends of structural variation on the position of  $\text{C}=\text{O}$  stretching frequencies may be summarized as follows:

1. The more electronegative the group X in the system  $\text{R}-\text{CO}-\text{X}-$ , the higher is the frequency.
2.  $\alpha, \beta$  Unsaturation causes a lowering of frequency of  $15$  to  $40 \text{ cm}^{-1}$ , except in amides, where little shift is observed and that usually to higher frequency.
3. Further conjugation has relatively little effect.
4. Ring strain in cyclic compounds causes a relatively large shift to higher frequency. This phenomenon provides a remarkably reliable test of ring size, distinguishing clearly between four-, five-, and larger-membered-ring ketones, lactones, and lactams. Six-ring and larger ketones, lactones, and lactams show the normal frequency found for the open-chain compounds.
5. Hydrogen bonding to a carbonyl group causes a shift to lower frequency of  $40$  to  $60 \text{ cm}^{-1}$ . Acids, amides, enolized  $\beta$ -keto carbonyl systems, and *o*-hydroxyphenol and *o*-aminophenyl carbonyl compounds show this effect. All carbonyl compounds tend to give slightly lower values for the carbonyl stretching frequency in the solid state compared with the value for dilute solutions.
6. Where more than one of the structural influences on a particular carbonyl group is operating, the net effect is usually close to additive.

**TABLE 7.24** Absorption Frequencies of Other Double Bonds*Abbreviations Used in the Table*

m, moderately strong                      vs, very strong  
 m-s, moderate to strong                w, weak  
 var, of variable strength

| Group                                                                                                   | Band, $\text{cm}^{-1}$                                                                                   | Remarks                                                                                     |
|---------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| Alkenes $\text{>C=C<}$                                                                                  |                                                                                                          |                                                                                             |
| Nonconjugated                                                                                           | 1680–1620 (w-m)                                                                                          | May be very weak if symmetrically substituted                                               |
| Conjugated with aromatic ring                                                                           | 1640–1610 (m)                                                                                            | More intense than with unconjugated double bonds                                            |
| Internal (ring)<br><br>Carbons: $n = 3$<br>$n = 4$<br>$n = 5$<br><br>$n \geq 6$                         | 3060–2995 (m)<br><br>ca 1665 (w-m)<br>ca 1565 (w-m)<br>ca 1610 (w-m)<br>1370–1340 (s)<br>1650–1645 (w-m) | Highest frequencies for smallest ring<br><br><br><br>Characteristic                         |
| Exocyclic $\text{C}=\text{C}(\text{CH}_2)_n$ $n = 2$<br>$n = 3$<br>$n \geq 4$                           | 1780–1730 (m)<br>ca 1680 (m)<br>1655–1650 (m)                                                            |                                                                                             |
| Fulvene                | 1645–1630 (m)<br><br>1370–1340 (s)<br>790–765 (s)                                                        |                                                                                             |
| Dienes, trienes, etc.                                                                                   | 1650 (s)<br>and 1600 (s)                                                                                 | Lower-frequency band usually more intense and may hide or overlap the higher-frequency band |
| $\alpha,\beta$ -Unsaturated carbonyl compounds                                                          | 1640–1590 (m)                                                                                            | Usually much weaker than the $\text{C}=\text{O}$ band                                       |
| Enol esters, enol ethers, and enamines                                                                  | 1700–1650 (s)                                                                                            |                                                                                             |
| Imines, oximes, and amidines $\text{>C=N-}$                                                             |                                                                                                          |                                                                                             |
| Imines and oximes<br>Aliphatic<br>$\alpha,\beta$ -Unsaturated and aromatic<br>Conjugated cyclic systems | 1690–1640 (w)<br>1650–1620 (m)<br>1660–1480 (var)<br>960–930 (s)                                         | NO stretching of oximes                                                                     |
| Imino ethers $\text{—O—C=N—}$                                                                           | 1690–1640 (var)                                                                                          | Usually a strong doublet                                                                    |

**TABLE 7.24** Absorption Frequencies of Other Double Bonds (*Continued*)

| Group                                                                                                                    | Band, $\text{cm}^{-1}$                                                   | Remarks                                                                                                                                                                                                                                              |
|--------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Imines, oximes, and amidines $\text{>C=N—}$ ( <i>continued</i> )                                                         |                                                                          |                                                                                                                                                                                                                                                      |
| Imino thioethers $\text{—S—C=N=}$                                                                                        | 1640–1605 (var)                                                          |                                                                                                                                                                                                                                                      |
| Imine oxides $\text{>C=N}^+\text{—}\bar{\text{O}}$                                                                       | 1620–1550 (s)                                                            |                                                                                                                                                                                                                                                      |
| Amidines $\text{>N—C=N—}$                                                                                                | 1685–1580 (var)                                                          |                                                                                                                                                                                                                                                      |
| Benzamidines Aryl—C=N—N                                                                                                  | 1630–1590                                                                |                                                                                                                                                                                                                                                      |
| Guanidine $\begin{array}{c} \text{>N—C=N—} \\   \\ \text{N} \end{array}$                                                 | 1725–1625 (s)                                                            |                                                                                                                                                                                                                                                      |
| Azines $\text{>C=N—N=C<}$                                                                                                | 1670–1600                                                                |                                                                                                                                                                                                                                                      |
| Hydrazoketones<br>$\text{—CO—C=N—N}$                                                                                     | 1600–1530 (vs)                                                           |                                                                                                                                                                                                                                                      |
| Azo compounds $\text{—N=N—}$                                                                                             |                                                                          |                                                                                                                                                                                                                                                      |
| Azo $\text{—N=N—}$<br>Aliphatic<br>Aromatic<br><i>cis</i><br><i>trans</i>                                                | ca 1575 (var)<br><br>ca 1510 (w)<br>1440–1410 (w)                        | Very weak or inactive                                                                                                                                                                                                                                |
| Azoxy $\begin{array}{c} \text{—}\overset{+}{\text{N}}=\text{N—} \\   \\ \text{O}^- \end{array}$<br>Aliphatic<br>Aromatic | 1590–1495 (m–s)<br>1345–1285 (m–s)<br>1480–1450 (m–s)<br>1340–1315 (m–s) |                                                                                                                                                                                                                                                      |
| Azothio $\text{—N}=\overset{+}{\text{N}}\text{—}\bar{\text{S}}\text{—}$                                                  | 1465–1445 (w)<br>1070–1055 (w)                                           |                                                                                                                                                                                                                                                      |
| Nitro compounds $\text{N=O}$                                                                                             |                                                                          |                                                                                                                                                                                                                                                      |
| Nitro $\text{C—NO}_2$<br>Aliphatic                                                                                       | ca 1560 (s)<br>1385–1350 (s)                                             | The two bands are due to asymmetrical and symmetrical stretching of the $\text{N=O}$ bond. Electron-withdrawing substituents adjacent to nitro group increase the frequency of the asymmetrical band and decrease that of the symmetrical frequency. |

**TABLE 7.24** Absorption Frequencies of Other Double Bonds (*Continued*)

| Group                                                                    | Band, $\text{cm}^{-1}$                                                             | Remarks                                                                                                                                                                                      |
|--------------------------------------------------------------------------|------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Nitro compounds $\text{N}=\text{O}$ ( <i>continued</i> )                 |                                                                                    |                                                                                                                                                                                              |
| Nitro $\text{C}-\text{NO}_2$ ( <i>continued</i> )                        |                                                                                    |                                                                                                                                                                                              |
| Aromatic                                                                 | 1570–1485 (s)<br>1380–1320 (s)                                                     | See above remark; also bulky orthosubstituents shift band to higher frequencies. Strong H bonding shifts frequency to lower end of range.<br>Strong and sometimes at ca 750 $\text{cm}^{-1}$ |
|                                                                          | 865–835 (s)                                                                        |                                                                                                                                                                                              |
| $\alpha,\beta$ -Unsaturated Nitroalkenes                                 | 580–520 (var)<br>1530–1510 (s)<br>1360–1335 (s)                                    |                                                                                                                                                                                              |
|                                                                          |                                                                                    |                                                                                                                                                                                              |
| Nitrates $-\text{O}-\text{NO}_2$                                         | 1650–1625 (vs)<br>1285–1275 (vs)<br>870–855 (vs)<br>760–755 (w–m)<br>710–695 (w–m) |                                                                                                                                                                                              |
| Nitramines $\text{>N}-\text{NO}_2$                                       | 1630–1550 (s)<br>1300–1250 (s)                                                     |                                                                                                                                                                                              |
| Nitrates $-\text{O}-\text{N}=\text{O}$                                   | 1680–1610 (vs)<br>815–750 (s)<br>850–810 (s)<br>690–615 (s)                        | Two bands<br><i>Trans</i> form<br><i>Cis</i> form                                                                                                                                            |
| Thionitrites $-\text{S}-\text{N}=\text{O}$                               | 730–685 (m–s)                                                                      |                                                                                                                                                                                              |
| Nitroso $\text{>C}-\text{N}=\text{O}$                                    | 1600–1500 (s)                                                                      |                                                                                                                                                                                              |
| $\text{N}-\overset{+}{\text{N}}=\bar{\text{O}}$<br>Aliphatic<br>Aromatic | 1530–1495 (m–s)<br>1480–1450 (m–s)<br>1335–1315 (m–s)                              |                                                                                                                                                                                              |
| Nitrogen oxides $\text{N}\rightarrow\text{O}$                            |                                                                                    |                                                                                                                                                                                              |
| Pyridine                                                                 | 1320–1230 (m–s)<br>1190–1150 (m–s)                                                 | Affected by ring substituents                                                                                                                                                                |
| Pyrazine                                                                 | 1380–1280 (m–s)<br>1040–990 (m–s)<br>ca 850 (m)                                    |                                                                                                                                                                                              |
|                                                                          |                                                                                    |                                                                                                                                                                                              |

**TABLE 7.25** Absorption Frequencies of Aromatic Bands*Abbreviations Used in the Table*

m, moderately strong

var, of variable strength

m-s, moderate to strong

w-m, weak to moderately strong

s, strong

| Group                 | Band, $\text{cm}^{-1}$                                                        | Remarks                                                                                                                                 |
|-----------------------|-------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Aromatic rings        | ca 1600 (m)<br>ca 1580 (m)<br>ca 1470 (m)<br>ca 1510 (m)                      | Stronger when ring is further conjugated<br>When substituent on ring is electron acceptor<br>When substituent on ring is electron donor |
| Five adjacent H       | 900–860 (w-m)<br>770–730 (s)<br>720–680 (s)<br>625–605 (w-m)<br>ca 550 (w-m)  | Substituents: $\text{C}=\text{C}$ , $\text{C}\equiv\text{C}$ , $\text{C}\equiv\text{N}$                                                 |
| 1,2-Substitution      | 770–735 (s)<br>555–495 (w-m)<br>470–415 (m-s)                                 |                                                                                                                                         |
| 1,3-Substitution      | 810–750 (s)<br>560–505 (m)<br>460–415 (m-s)                                   | 490–460 $\text{cm}^{-1}$ when substituents are electron-accepting groups                                                                |
| 1,4-Substitution      | 860–800 (s)<br>650–615 (w-m)<br>520–440 (m-s)                                 | 520–490 $\text{cm}^{-1}$ when substituents are electron-donating groups                                                                 |
| 1,2,3-Trisubstitution | 800–760 (s)<br>720–685 (s)<br>570–535 (s)<br>ca 485                           |                                                                                                                                         |
| 1,2,4-Trisubstitution | 900–885 (m)<br>780–760 (s)<br>475–425 (m-s)                                   |                                                                                                                                         |
| 1,3,5-Trisubstitution | 950–925 (var)<br>865–810 (s)<br>730–680 (m-s)<br>535–495 (s)<br>470–450 (w-m) |                                                                                                                                         |
| Pentasubstitution     | 900–860 (m-s)<br>580–535 (s)                                                  |                                                                                                                                         |
| Hexasubstitution      | 415–385 (m-s)                                                                 |                                                                                                                                         |



**TABLE 7.26** Absorption Frequencies of Miscellaneous Bands*Abbreviations Used in the Table*

|                           |                                |
|---------------------------|--------------------------------|
| m, moderately strong      | vs, very strong                |
| m-s, moderate to strong   | w, weak                        |
| s, strong                 | w-m, weak to moderately strong |
| var, of variable strength |                                |

| Group                                                                                                 | Band, cm <sup>-1</sup>                                                        | Remarks                                                                                                                                                     |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ethers                                                                                                |                                                                               |                                                                                                                                                             |
| Saturated aliphatic<br>$\geq\text{C}-\text{O}-\text{C}\leq$                                           | 1150–1060 (vs)<br><br>1140–900 (s)                                            | Two peaks may be observed for branched chain, usually 1140–1110 cm <sup>-1</sup> .<br>Usually 930–900 cm <sup>-1</sup> ; may be absent for symmetric ethers |
| Alkyl-aryl<br>$\begin{array}{c} \text{=C}-\text{O}-\text{C}\leq \\   \end{array}$                     | 1270–1230 (vs)<br>1120–1020 (s)                                               | $\text{=CO}$ stretching<br>CO stretching                                                                                                                    |
| Vinyl                                                                                                 | 1225–1200 (s)                                                                 | Usually about 1205 cm <sup>-1</sup>                                                                                                                         |
| Diaryl<br>$\begin{array}{c} \text{=C}-\text{O}-\text{C=} \\   \quad   \end{array}$                    | 1200–1120 (s)<br>1100–1050 (s)                                                |                                                                                                                                                             |
| Cyclic                                                                                                | 1270–1030 (s)                                                                 |                                                                                                                                                             |
| Epoxides<br>$\begin{array}{c} \text{>C} \quad \text{C}< \\ \diagdown \quad / \\ \text{O} \end{array}$ | 1260–1240 (m-s)<br>880–805 (m)<br>950–860 (var)<br>865–785 (m)<br>770–750 (m) | Monosubstituted<br><i>Trans</i> form<br><i>Cis</i> form<br>Trisubstituted                                                                                   |
| Ketals and acetals                                                                                    | 1190–1140 (s)<br>1195–1125 (s)<br>1100–1000 (s)<br>1060–1035 (s)              | Strongest band<br>Sometimes obscured                                                                                                                        |
| Phthalanes                                                                                            | 915–895 (s)                                                                   |                                                                                                                                                             |
| Aromatic methylenedioxy                                                                               | 1265–1235 (s)                                                                 |                                                                                                                                                             |
| Peroxides                                                                                             |                                                                               |                                                                                                                                                             |
| $-\text{O}-\text{O}-$                                                                                 | 900–830 (w)<br>1150–1030 (m-s)<br>ca 1000 (m)                                 | Alkyl<br>Aryl                                                                                                                                               |

**TABLE 7.26** Absorption Frequencies of Miscellaneous Bands (*Continued*)

| Group                                                                                                         | Band, $\text{cm}^{-1}$                                                                              | Remarks                                                                                                                                            |
|---------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| Sulfur compounds                                                                                              |                                                                                                     |                                                                                                                                                    |
| Thiols<br>$\text{—S—H}$<br>$\text{—CO—SH}$<br>$\text{—CS—SH}$                                                 | 2600–2450 (w)<br>840–830 (m)<br>ca 860 (s)                                                          | Broad                                                                                                                                              |
| Thiocarbonyl<br>$\text{>C=S}$<br><br>$\text{>N—C=S}$<br>$\quad \quad  $<br>$\text{—S—C=S}$<br>$\quad \quad  $ | 1200–1050 (s)<br><br>1570–1395<br>1420–1260<br>1140–940<br>ca 580 (s)                               | Behaves generally in manner similar to carbonyl band                                                                                               |
| Sulfoxides<br>$\text{>S=O}$                                                                                   | 1075–1040 (vs)<br><br>730–690 (var)<br>395–360 (var)                                                | Halogen or oxygen atom bonded to sulfur increases the frequency.                                                                                   |
| Sulfones<br>$\text{>SO}_2$                                                                                    | 1360–1290 (vs)<br><br>1170–1120 (vs)<br>610–545 (m–s)<br>525–495 (m–s)                              | Halogen or oxygen atom bonded to sulfur increases the frequency.                                                                                   |
| Sulfonamides<br>$\text{—SO}_2\text{—N<}$                                                                      | 1380–1330 (vs)<br>1170–1140 (vs)<br>950–860 (m)<br>715–700 (w–m)                                    |                                                                                                                                                    |
| Sulfonates<br>$\text{—SO}_2\text{—O—}$                                                                        | 1420–1330 (s)<br>1200–1145 (s)                                                                      | May appear as doublet                                                                                                                              |
| Thiosulfonates<br>$\text{—SO}_2\text{—S—}$                                                                    | ca 1340 (vs)                                                                                        |                                                                                                                                                    |
| Sulfates $\text{—O—SO}_2\text{—O—}$<br><br>Primary alkyl salts<br><br>Secondary alkyl salts                   | 1415–1380 (s)<br>1200–1185 (s)<br>1315–1220 (s)<br>1140–1075 (m)<br>1270–1210 (vs)<br>1075–1050 (s) | Electronegative substituents increase frequencies.<br>Strongly influenced by metal ion<br><br>Doublet; both bands strongly influenced by metal ion |

TABLE 7.26 Absorption Frequencies of Miscellaneous Bands (Continued)

| Group                                                                                                                                                                                                                                                                                                                                        | Band, cm <sup>-1</sup>                                                                                                                                                                                                                                                                                | Remarks                                                                                      |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|
| Sulfur compounds (continued)                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                       |                                                                                              |
| <b>Stretching frequencies of C—S and S—S bonds</b><br>—S—CH <sub>3</sub><br>—S—CH <sub>2</sub> —<br>—S—CH<<br>—S—C≡<br>—S—aryl<br><br>R—S—S—R<br><br>Aryl—S—S—aryl<br>Polysulfides<br>CH <sub>2</sub> —S—CH <sub>2</sub> —<br>(R—S) <sub>2</sub> C=O<br><br>—CO—S—<br>—CS—S<br><div><div><div>S—</div><div>=C</div><div>S—</div></div></div> | 710–685 (w–m)<br>660–630 (w–m)<br>630–600 (w–m)<br>600–570 (w–m)<br>1110–1070 (m)<br>710–685 (w–m)<br>705–570 (w)<br>520–500 (w)<br>500–430 (w–m)<br>500–470 (w–m)<br>695–655 (w–m)<br>880–825 (s)<br>570–560 (var)<br>1035–935 (s)<br>ca 580 (s)<br>1050–900 (m–s)<br>980–850 (m–s)<br>900–800 (m–s) | CSC stretching<br><br><br><br><br><br><br><br><br><br><br>Monoionic<br>Ionic 1,1-dithiolates |
| Phosphorus compounds                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                       |                                                                                              |
| P—H                                                                                                                                                                                                                                                                                                                                          | 2455–2265 (m)<br><br>1150–965 (w–m)                                                                                                                                                                                                                                                                   | Sharp. Phosphines lie in the region 2285–2265 cm <sup>-1</sup> .                             |
| —PH <sub>2</sub>                                                                                                                                                                                                                                                                                                                             | 1100–1085 (m)<br>1065–1040 (w–m)<br>940–910 (m)                                                                                                                                                                                                                                                       |                                                                                              |
| P—alkyl                                                                                                                                                                                                                                                                                                                                      | 795–650 (m–s)                                                                                                                                                                                                                                                                                         |                                                                                              |
| P—aryl                                                                                                                                                                                                                                                                                                                                       | 1130–1090 (s)<br>750–680 (s)                                                                                                                                                                                                                                                                          |                                                                                              |
| P—O—alkyl                                                                                                                                                                                                                                                                                                                                    | 1050–970 (s)                                                                                                                                                                                                                                                                                          | Broad                                                                                        |
| P—O—aryl                                                                                                                                                                                                                                                                                                                                     | 1240–1190 (s)                                                                                                                                                                                                                                                                                         |                                                                                              |
| P—O—P                                                                                                                                                                                                                                                                                                                                        | 970–910                                                                                                                                                                                                                                                                                               | Broad                                                                                        |
| P=O                                                                                                                                                                                                                                                                                                                                          | 1350–1150 (s)                                                                                                                                                                                                                                                                                         | May appear as doublet                                                                        |
| <div><div><div>O</div><div>P=</div><div>OH</div></div></div>                                                                                                                                                                                                                                                                                 | 2725–2520 (w–m)<br>2350–2080 (w–m)<br>1740–1600 (w–m)<br>1335 (s)<br>1090–910 (s)<br>540–450 (w–m)                                                                                                                                                                                                    | H-bonded; broad<br>Broad; may be doublet for aryl acids<br><br>P=O stretching                |

**TABLE 7.26** Absorption Frequencies of Miscellaneous Bands (*Continued*)

| Group                                                                                                    | Band, $\text{cm}^{-1}$                                                                                                      | Remarks                                                                                                                                                 |
|----------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| Phosphorus compounds ( <i>continued</i> )                                                                |                                                                                                                             |                                                                                                                                                         |
| $\text{P}=\text{S}$                                                                                      | 865–655 (m–s)<br>595–530 (var)                                                                                              |                                                                                                                                                         |
| $\begin{array}{c} \text{S} \\ \parallel \\ \text{P} \\ \diagup \quad \diagdown \\ \text{OH} \end{array}$ | 3100–3000 (w)<br>2360–2200 (w)<br>935–910 (s)<br>810–750 (m–s)<br>655585 (var)                                              | PO stretching<br>P=S stretching<br>P=S stretching                                                                                                       |
| Silicon compounds                                                                                        |                                                                                                                             |                                                                                                                                                         |
| $\text{Si}-\text{H}$                                                                                     | 2250–2100 (s)<br>985–800                                                                                                    | $\text{SiH}_3$ has two bands.                                                                                                                           |
| $\text{Si}-\text{C}$                                                                                     | 860–760                                                                                                                     | Accompanied by $\text{CH}_2$ rocking                                                                                                                    |
| $\text{Si}-\text{C}\equiv$                                                                               | 1280–1250 (s)                                                                                                               | Sharp                                                                                                                                                   |
| $\text{Si}-\text{C}_2\text{H}_5$                                                                         | 1250–1220 (m)<br>1020–1000 (m)<br>970–945 (m)                                                                               |                                                                                                                                                         |
| $\text{Si}-\text{Aryl}$                                                                                  | 1125–1090 (vs)                                                                                                              | Splits into two bands when two aryl groups are attached to one silicon atom, but has only one band when three aryl groups attached                      |
| $\equiv\text{Si}-\text{OH}$                                                                              | 870–820                                                                                                                     | OH deformation band                                                                                                                                     |
| $\equiv\text{Si}-\text{O}-\text{Si}\equiv$                                                               | 1100–1000                                                                                                                   |                                                                                                                                                         |
| $\equiv\text{Si}-\text{N}-\text{Si}\equiv$                                                               | 940–870 (s)                                                                                                                 |                                                                                                                                                         |
| $\equiv\text{Si}-\text{Cl}$                                                                              | 550–470 (s)<br>250–150                                                                                                      |                                                                                                                                                         |
| $\triangleright\text{SiCl}_2$                                                                            | 595–535 (s)<br>540–460 (m)                                                                                                  |                                                                                                                                                         |
| $-\text{SiCl}_3$                                                                                         | 625–570 (s)<br>535–450 (m)                                                                                                  |                                                                                                                                                         |
| Boron compounds                                                                                          |                                                                                                                             |                                                                                                                                                         |
| Boranes<br>$\triangleright\text{BH}$ or $-\text{BH}_2$                                                   | 2640–2450 (m–s)<br>2640–2570 (m–s)<br>2535–2485 (m–s)<br>2380–2315 (s)<br>2285–2265 (s)<br>2140–2080 (w–m)<br>2580–2450 (m) | Free H in BH<br>Free H in $\text{BH}_2$ plus second band<br><br>In complexes; second band for $\text{BH}_2$<br><br>Bridged H<br>Borazoles and borazines |

**TABLE 7.26** Absorption Frequencies of Miscellaneous Bands (*Continued*)

| Group                                                                            | Band, cm <sup>-1</sup>                                                                                                              | Remarks                                                                          |
|----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|
| Boron compounds ( <i>continued</i> )                                             |                                                                                                                                     |                                                                                  |
| BH <sub>4</sub> <sup>-</sup>                                                     | 2310–2195 (s)                                                                                                                       | Two bands                                                                        |
| B—N                                                                              | 1550–1330<br>750–635                                                                                                                | Borazines and borazoles                                                          |
| B—O                                                                              | 1390–1310 (s)<br>1280–1200                                                                                                          | BO stretching<br>Metal orthoborates                                              |
| B—Cl<br>B—Br                                                                     | 1090–890 (s)                                                                                                                        | Plus other bands at lower frequencies<br>for BX <sub>2</sub> and BX <sub>3</sub> |
| B—F                                                                              | 1500–840 (var)                                                                                                                      | Isotope splitting present                                                        |
| XBF <sub>2</sub>                                                                 | 1500–1410 (s)<br>1300–1200 (s)                                                                                                      |                                                                                  |
| X <sub>2</sub> BF                                                                | 1360–1300 (s)                                                                                                                       |                                                                                  |
| BF <sub>3</sub> complexes                                                        | 1260–1125 (s)<br>1030–800 (s)                                                                                                       | Band splitting may be added to isotopic<br>splittings.                           |
| BF <sub>4</sub> <sup>-</sup>                                                     | ca 1030 (vs)                                                                                                                        |                                                                                  |
| Halogen compounds                                                                |                                                                                                                                     |                                                                                  |
| C—F<br>Aliphatic, mono-F<br><br>Aliphatic, di-F<br>Aliphatic, poly-F<br>Aromatic | 1110–1000 (vs)<br>780–680 (s)<br>1250–1050 (vs)<br>1360–1090 (vs)<br>1270–1100 (m)<br>680–520 (m–s)<br>420–375 (var)<br>340–240 (s) | Two bands<br>Number of bands                                                     |
| —CF <sub>3</sub><br>Aliphatic<br><br><br>Aromatic                                | 1350–1120 (vs)<br>780–680 (s)<br>680–590 (s)<br>600–540 (s)<br>555–505 (s)<br>1330–1310 (m–s)<br>600–580 (s)                        |                                                                                  |
| C—Cl<br>Primary alkanes                                                          | 730–720 (s)<br>685–680 (s)<br>660–650 (s)                                                                                           |                                                                                  |

**TABLE 7.26** Absorption Frequencies of Miscellaneous Bands (*Continued*)

| Group                                  | Band, cm <sup>-1</sup>                        | Remarks |
|----------------------------------------|-----------------------------------------------|---------|
| Halogen compounds ( <i>continued</i> ) |                                               |         |
| C—Cl ( <i>continued</i> )              |                                               |         |
| Secondary alkanes                      | ca 760 (m)<br>675–655 (m–s)<br>615–605 (s)    |         |
| Tertiary alkanes                       | 635–610 (m–s)<br>580–560 (m–s)                |         |
| Poly-Cl                                | 800–700 (vs)                                  |         |
| Aryl:                                  |                                               |         |
| 1,2-                                   | 1060–1035 (m)                                 |         |
| 1,3-                                   | 1080–1075 (m)                                 |         |
| 1,4-                                   | 1100–1090 (m)                                 |         |
| Chloroformates                         | ca 690 (s)<br>485–470 (s)                     |         |
| Axial Cl                               | 730–580 (s)                                   |         |
| Equatorial Cl                          | 780–740 (s)                                   |         |
| C—Br                                   |                                               |         |
| Primary alkanes                        | 645–635 (s)<br>565–555 (s)<br>440–430 (var)   |         |
| Secondary alkanes                      | 620–605 (s)<br>590–575 (m–w)<br>540–530 (s)   |         |
| Tertiary alkanes                       | 600–595 (m–s)<br>525–505 (s)                  |         |
| Axial                                  | 690–550 (s)                                   |         |
| Equatorial                             | 750–685 (s)                                   |         |
| Aryl:                                  |                                               |         |
| 1,2-                                   | 1045–1025 (m)                                 |         |
| 1,3-; 1,4-                             | 1075–1065 (m)                                 |         |
| Other bands                            | 400–260 (s)<br>325–175 (m–s)<br>290–225 (m–s) |         |
| C—I                                    |                                               |         |
| Primary alkanes                        | 600–585 (s)<br>515–500 (s)                    |         |
| Secondary alkanes                      | ca 575 (s)<br>550–520 (s)<br>490–480 (s)      |         |
| Tertiary alkanes                       | 580–560 (s)<br>510–485 (m)<br>485–465 (s)     |         |
| Aromatic                               | 1060–1055 (m–s)<br>310–160 (s)<br>265–185     |         |
| Axial                                  | ca 640 (s)                                    |         |
| Equatorial                             | ca 655 (s)                                    |         |

**TABLE 7.26** Absorption Frequencies of Miscellaneous Bands (*Continued*)

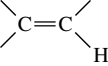
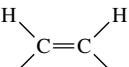
| Group            | Band, cm <sup>-1</sup>                        | Remarks                   |
|------------------|-----------------------------------------------|---------------------------|
| Inorganic ions   |                                               |                           |
| Ammonium         | 3300–3030                                     | Several bands, all strong |
| Cyanate          | 2220–2130 (s)                                 |                           |
| Cyanide          | 2200–2000                                     |                           |
| Carbonate        | 1450–1410                                     |                           |
| Hydrogen sulfate | 1190–1160 (s)<br>1180–1000 (s)<br>880–840 (m) |                           |
| Nitrate          | 1410–1350 (vs)<br>860–800 (m)                 |                           |
| Nitrite          | 1275–1230 (s)<br>835–800 (m)                  | Shoulder                  |
| Phosphate        | 1100–1000                                     |                           |
| Sulfate          | 1130–1080 (s)                                 |                           |
| Thiocyanate      | ca 2050 (s)                                   |                           |

**TABLE 7.27** Absorption Frequencies in the Near Infrared

*Values in parentheses are molar absorptivity.*

| Class                                                 | Band, cm <sup>-1</sup>                                                  | Remarks                               |
|-------------------------------------------------------|-------------------------------------------------------------------------|---------------------------------------|
| Acetylenes                                            | 9800–9430<br>6580–6400 (1.0)                                            | Overtone of ≡CH stretching            |
| Alcohols (nonhydrogen-bonded)                         | 7140–7010 (2.0)                                                         | Overtone of OH stretching             |
| Aldehydes<br>Aliphatic<br><br>Aromatic<br><br>Formate | 4640–4520 (0.5)<br><br>ca 8000<br>ca 4525<br>ca 4445<br>4775–4630 (1.0) | Combination of C=O and CH stretchings |

**TABLE 7.27** Absorption Frequencies in the Near Infrared (*Continued*)

| Class                                                                                                                                     | Band, cm <sup>-1</sup>                                                    | Remarks                                                                                                                                                                                                       |
|-------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Alkanes<br>—CH <sub>3</sub>                                                                                                               | 9000–8350 (0.02)<br>5850–5660 (0.1)<br>4510–4280 (0.3)                    | All bands very weak                                                                                                                                                                                           |
| —CH <sub>2</sub> —                                                                                                                        | 9170–8475 (0.02)<br>5830–6640 (0.1)<br>4420–4070 (0.25)                   |                                                                                                                                                                                                               |
| ≡CH                                                                                                                                       | 8550–8130<br>7000–6800<br>5650–5560                                       |                                                                                                                                                                                                               |
| Cyclopropane                                                                                                                              | 6160–6060<br>4500–4400                                                    |                                                                                                                                                                                                               |
| Alkenes<br><br>≥C=CH <sub>2</sub> and —CH=CH <sub>2</sub> | 6850–6370 (1.0)<br>7580–7300 (0.02)<br>6140–5980 (0.2)<br>4760–4700 (1.2) | <i>Trans</i> isomers have no unique bands.                                                                                                                                                                    |
|                                                           | 4760–4660 (0.15)                                                          |                                                                                                                                                                                                               |
| —O—CH=CH <sub>2</sub>                                                                                                                     | 6250–6040 (0.3)                                                           |                                                                                                                                                                                                               |
| —CO—CH=CH <sub>2</sub>                                                                                                                    | 7580–7410 (0.02)<br>6190–5990 (0.3)<br>4820–4750 (0.2–0.5)                |                                                                                                                                                                                                               |
| Amides<br>Primary                                                                                                                         | 7400–6540 (0.7)<br>5160–5060 (3.0)<br>5040–4990 (0.5)<br>4960–4880 (0.5)  | Two bands; overtone of NH stretch<br>Second overtone of C=O stretch;<br>second overtone of NH deformation;<br>combination of C=O and NH<br>Overtone of NH stretch<br>Combination of NH stretch and NH bending |
| Secondary                                                                                                                                 | 7330–7140 (0.5)<br>5050–4960 (0.4)                                        |                                                                                                                                                                                                               |
| Amines, aliphatic<br>Primary                                                                                                              | 9710–9350<br>6670–6450 (0.5)<br>5075–4900 (0.7)                           | Second overtone of NH stretch<br>Two bands; overtone of NH stretch<br>Two bands; combination of NH stretch and NH bending<br>Second overtone of NH stretch<br>Overtone of NH stretch                          |
| Secondary                                                                                                                                 | 9800–9350<br>6580–6410 (0.5)                                              |                                                                                                                                                                                                               |
| Amines, aromatic<br>Primary                                                                                                               | 9950–9520 (0.4)<br>7040–6850 (0.2)<br>6760–6580 (1.4)<br>5140–5040 (1.5)  |                                                                                                                                                                                                               |
| Secondary                                                                                                                                 | 10 000–9710<br>6800–6580 (0.5)                                            |                                                                                                                                                                                                               |



**TABLE 7.27** Absorption Frequencies in the Near Infrared (*Continued*)

| Class                                               | Band, $\text{cm}^{-1}$                                                   | Remarks                           |
|-----------------------------------------------------|--------------------------------------------------------------------------|-----------------------------------|
| Aryl-H                                              | 7660–7330 (0.1)<br>6170–5880 (0.1)                                       | Overtone of CH stretch            |
| Carbonyl                                            | 5200–5100                                                                |                                   |
| Carboxylic acids                                    | 7000–6800                                                                |                                   |
| Epoxide (terminal)                                  | 6135–5960 (0.2)<br>4665–4520 (1.2)                                       | Cyclopropane bands in same region |
| Glycols                                             | 7140–7040                                                                |                                   |
| Hydroperoxides<br>Aliphatic<br><br>Aromatic         | 6940–6750 (2.0)<br>4960–4880 (0.8)<br>7040–6760 (1.0)<br>4950–4850 (1.3) | Two bands                         |
| Imides                                              | 9900–9620<br>6540–6370                                                   |                                   |
| Nitriles                                            | 5350–5200 (0.1)                                                          |                                   |
| Oximes                                              | 7140–7050                                                                |                                   |
| Phosphines                                          | 5350–5260 (0.2)                                                          |                                   |
| Phenols<br>Nonbonded<br><br>Intramolecularly bonded | 7140–6800 (3.0)<br>5000–4950<br>7000–6700                                |                                   |
| Thiols                                              | 5100–4950 (0.05)                                                         |                                   |

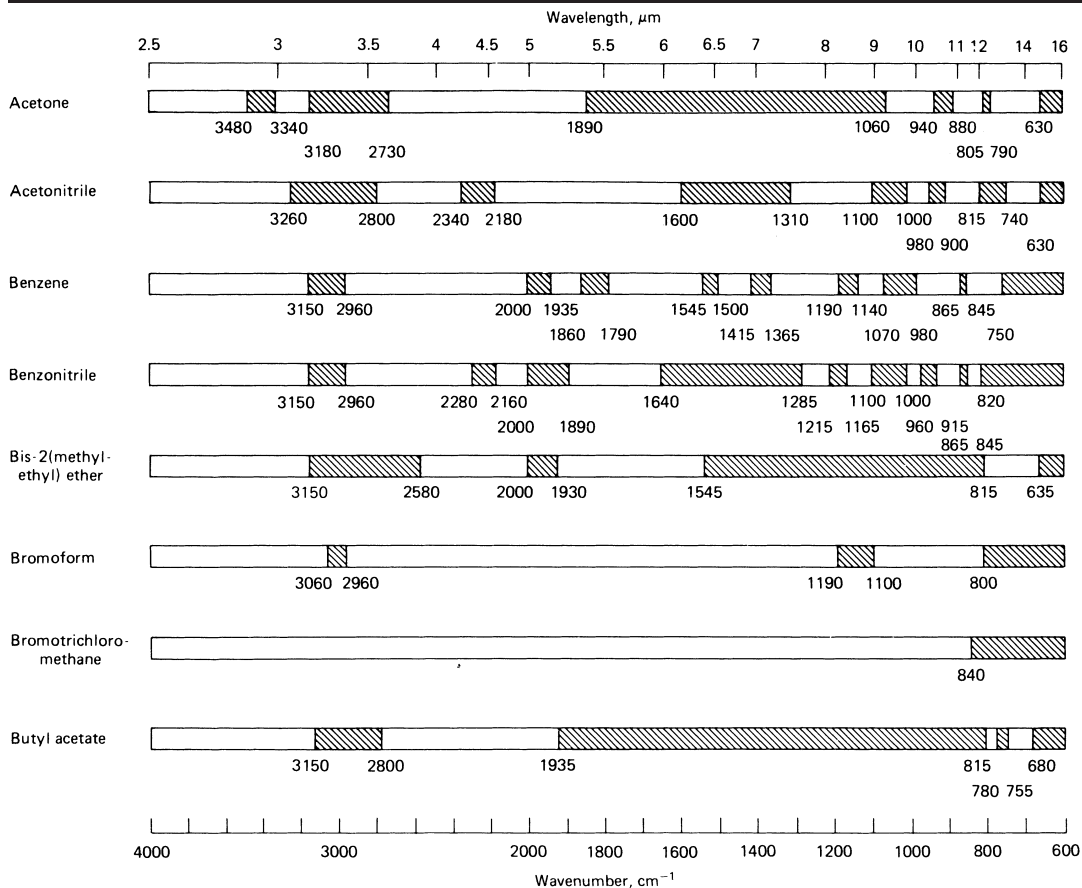
**TABLE 7.28** Infrared Transmitting Materials

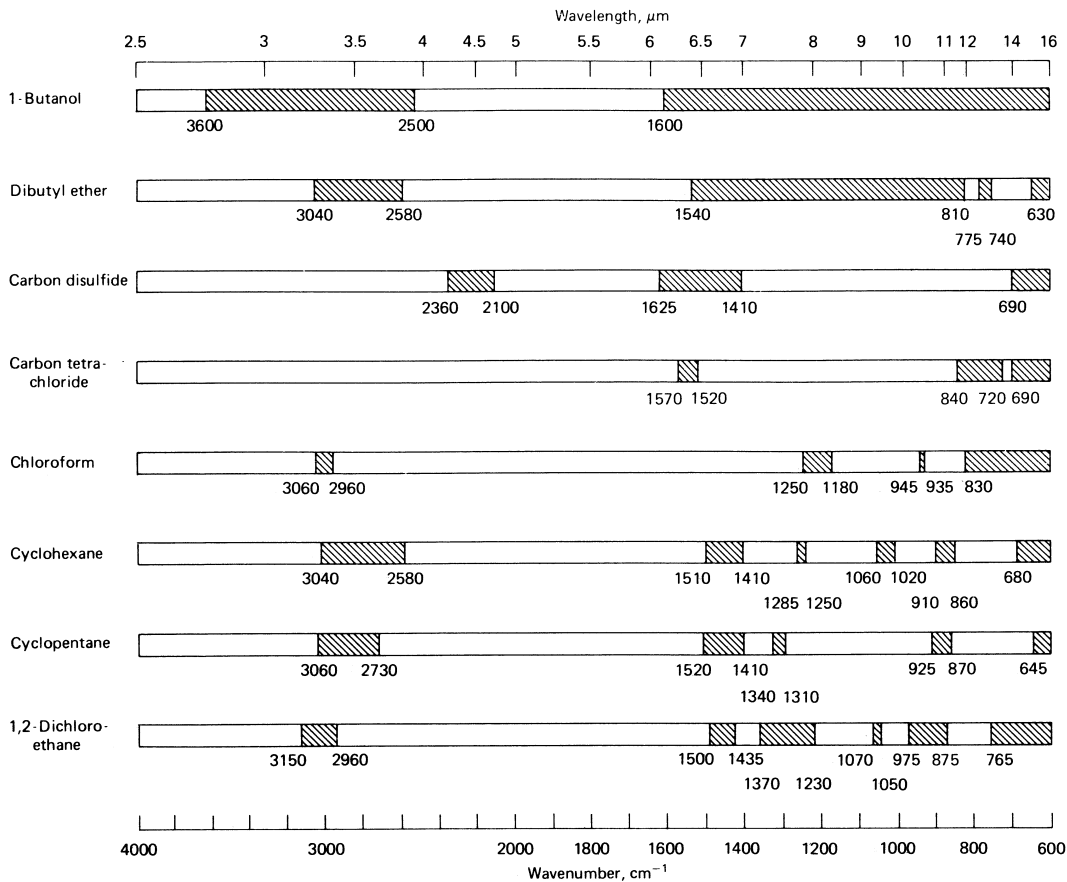
| Material                                              | Wavelength<br>range,<br>$\mu\text{m}$ | Wavenumber<br>range,<br>$\text{cm}^{-1}$ | Refractive<br>index at<br>$2\ \mu\text{m}$ |
|-------------------------------------------------------|---------------------------------------|------------------------------------------|--------------------------------------------|
| NaCl, rock salt                                       | 0.25–17                               | 40 000–590                               | 1.52                                       |
| KBr, potassium bromide                                | 0.25–25                               | 40 000–400                               | 1.53                                       |
| KCl, potassium chloride                               | 0.30–20                               | 33 000–500                               | 1.5                                        |
| AgCl, silver chloride*                                | 0.40–23                               | 25 000–435                               | 2.0                                        |
| AgBr, silver bromide*                                 | 0.50–35                               | 20 000–286                               | 2.2                                        |
| CaF <sub>2</sub> , calcium fluoride (Irtran-3)        | 0.15–9                                | 66 700–1 110                             | 1.40                                       |
| BaF <sub>2</sub> , barium fluoride                    | 0.20–11.5                             | 50 000–870                               | 1.46                                       |
| MgO, magnesium oxide (Irtran-5)                       | 0.39–9.4                              | 25 600–1 060                             | 1.71                                       |
| CsBr, cesium bromide                                  | 1–37                                  | 10 000–270                               | 1.67                                       |
| CsI, cesium iodide                                    | 1–50                                  | 10 000–200                               | 1.74                                       |
| TlBr-TlI, thallium bromide-iodide<br>(KRS-5)*         | 0.50–35                               | 20 000–286                               | 2.37                                       |
| ZnS, zinc sulfide (Irtran-2)                          | 0.57–14.7                             | 17 500–680                               | 2.26                                       |
| ZnSe, zinc selenide* (vacuum deposited)<br>(Irtran-4) | 1–18                                  | 10 000–556                               | 2.45                                       |
| CdTe, cadmium telluride (Irtran-6)                    | 2–28                                  | 5 000–360                                | 2.67                                       |
| Al <sub>2</sub> O <sub>3</sub> , sapphire*            | 0.20–6.5                              | 50 000–1538                              | 1.76                                       |
| SiO <sub>2</sub> , fused quartz                       | 0.16–3.7                              | 62 500–2 700                             |                                            |
| Ge, germanium*                                        | 0.50–16.7                             | 20 000–600                               | 4.0                                        |
| Si, silicon*                                          | 0.20–6.2                              | 50 000–1 613                             | 3.5                                        |
| Polyethylene                                          | 16–300                                | 625–33                                   | 1.54                                       |

\* Useful for internal reflection work.

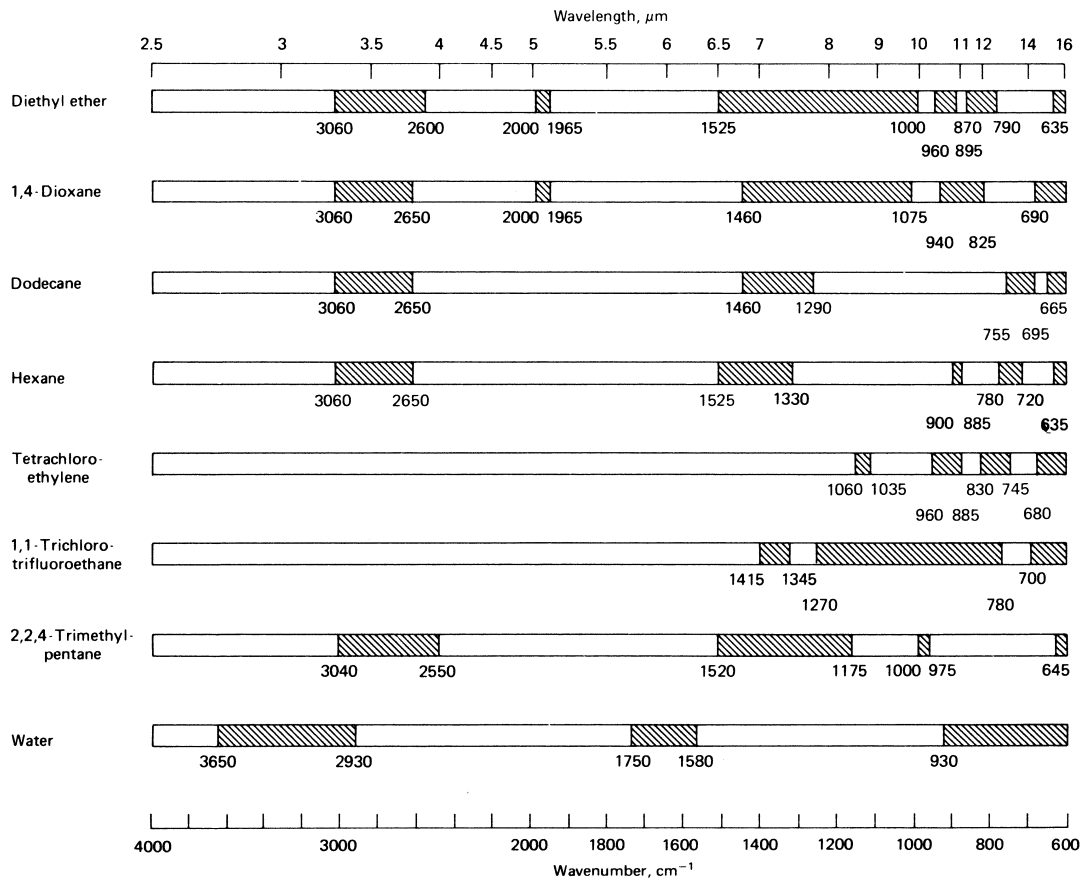
**TABLE 7.29** Infrared Transmission Characteristics of Selected Solvents

*Transmission below 80%, obtained with a 0.10-mm cell path, is shown as shaded area.*





**TABLE 7.29** Infrared Transmission Characteristics of Selected Solvents (*Continued*)



## 7.6 RAMAN SPECTROSCOPY

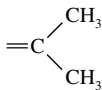
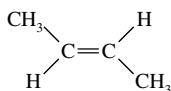
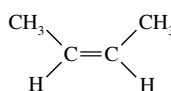
**TABLE 7.30** Raman Frequencies of Single Bonds to Hydrogen and Carbon

*Abbreviations Used in the Table*

|                               |                                |
|-------------------------------|--------------------------------|
| m, moderately strong          | vw, very weak                  |
| m-s, moderate to strong       | w, weak                        |
| m-vs, moderate to very strong | w-m, weak to moderately strong |
| s, strong                     | w-vs, weak to very strong      |
| vs, very strong               |                                |

| Group                              | Band, $\text{cm}^{-1}$                                                                                                    | Remarks                                                                                                                                           |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| Saturated C—H and C—C              |                                                                                                                           |                                                                                                                                                   |
| —CH <sub>3</sub>                   | 2969–2967 (s)<br>2884–2883 (s)<br>ca 1205 (s)<br>1150–1135<br>1060–1056<br>975–835 (s)<br>280–220                         | In aryl compounds<br>In unbranched alkyls<br>In unbranched alkyls<br>Terminal rocking of methyl group<br>CH <sub>2</sub> —CH <sub>3</sub> torsion |
| —CH <sub>2</sub> —                 | 2949–2912 (s)<br>2861–2849 (s)<br>1473–1443 (m-vs)<br>1305–1295 (s)<br>1140–1070 (m)<br>888–837 (w)<br>425–150<br>500–490 | Intensity proportional to number of CH <sub>2</sub> groups<br>Often two bands; see above<br><br>Substituent on aromatic ring                      |
| —CH(CH <sub>3</sub> ) <sub>2</sub> | 1350–1330 (m)<br>835–750 (s)                                                                                              | If attached to C=C bond, 870–800 $\text{cm}^{-1}$ . If attached to aryl ring, 740 $\text{cm}^{-1}$                                                |
| —C(CH <sub>3</sub> ) <sub>3</sub>  | 1265–1240 (m)<br>1220–1200 (m)<br>760–685 (vs)                                                                            | Not seen in <i>tert</i> -butyl bromide<br>Not seen in <i>tert</i> -butyl bromide<br>If attached to C=C or aromatic ring, 760–720 $\text{cm}^{-1}$ |
| Internal tertiary carbon atom      | 855–805 (w)<br>455–410                                                                                                    |                                                                                                                                                   |
| Internal quaternary carbon atom    | 710–680 (vs)<br>490–470                                                                                                   |                                                                                                                                                   |

**TABLE 7.30** Raman Frequencies of Single Bonds to Hydrogen and Carbon (*Continued*)

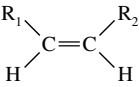
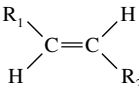
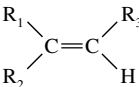
| Group                                                                              | Band, $\text{cm}^{-1}$                                                 | Remarks                                                                                                                                                                                                        |
|------------------------------------------------------------------------------------|------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Saturated C—H and C—C ( <i>continued</i> )                                         |                                                                        |                                                                                                                                                                                                                |
| Two adjacent tertiary carbon atoms                                                 | 730–920<br>770–725                                                     | Often a band at $530\text{--}524\text{ cm}^{-1}$ indicates presence of adjacent tertiary and quaternary carbon atoms.                                                                                          |
| Dialkyl substitution at $\alpha$ -carbon atom                                      | 800–700 (m–s)<br>680–650 (vs)<br>605–550                               |                                                                                                                                                                                                                |
| Cyclopropane                                                                       | 3101–3090<br>3038–3019<br>1210–1180 (s)                                | Shifts to $1200\text{ cm}^{-1}$ for monoalkyl or 1,2-dialkyl substitution and to $1320\text{ cm}^{-1}$ for <i>gem</i> -1,1-dialkyl substitution                                                                |
| Cyclobutane                                                                        | 1001–960 (vs)                                                          | Shifts to $933\text{ cm}^{-1}$ for monoalkyl, to $887\text{ cm}^{-1}$ for <i>cis</i> -1,3-dialkyl, and to $891\text{ cm}^{-1}$ plus $855\text{ cm}^{-1}$ (doublet) for <i>trans</i> -1,3,-dialkyl substitution |
| Cyclopentane                                                                       | 900–800 (s)                                                            |                                                                                                                                                                                                                |
| Cyclohexane                                                                        | 825–815 (vs)<br>810–795 (vs)                                           | Boat configuration<br>Chair configuration                                                                                                                                                                      |
| Cycloheptane                                                                       | ca 733                                                                 |                                                                                                                                                                                                                |
| Cyclooctane                                                                        | ca 703                                                                 |                                                                                                                                                                                                                |
|  | 1392–1377<br>450–400 (vw)<br>270–250 (m)                               |                                                                                                                                                                                                                |
|  | 1380–1379<br>492–455 (vw)<br>220–200 (m)                               |                                                                                                                                                                                                                |
|  | 1372–1368<br>970–952 (m)<br>592–545 (vw)<br>420–400 (m)<br>310–290 (m) |                                                                                                                                                                                                                |

**TABLE 7.30** Raman Frequencies of Single Bonds to Hydrogen and Carbon (*Continued*)

| Group                                                                                                                                                                        | Band, $\text{cm}^{-1}$                                   | Remarks                                                                                               |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Saturated C—H and C—C ( <i>continued</i> )                                                                                                                                   |                                                          |                                                                                                       |
| $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{CH}_3 \quad \text{H} \end{array}$        | 1385–1375<br>522–488 (w)                                 |                                                                                                       |
| $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$     | 1392–1386<br>690–678 (m–s)<br>510–485 (m)<br>424–388 (w) |                                                                                                       |
| $\begin{array}{c} \equiv\text{C}-\text{C}-\text{C}\equiv \\ \parallel \\ \text{O} \end{array}$                                                                               | 1170–1100 (w–m)<br>600–580 (m–s)                         |                                                                                                       |
| $\begin{array}{c} \equiv\text{C}-\text{C}- \\ \parallel \\ \text{O} \end{array}$                                                                                             | 1120–1090 (m–vs)<br><br>600–510 (w–m)                    | Tertiary or quaternary carbon adjacent to carbonyl group lowers the frequency $300 \text{ cm}^{-1}$ . |
| —CH <sub>2</sub> —CO—                                                                                                                                                        | 1420–1410 (s)                                            |                                                                                                       |
| —CHO                                                                                                                                                                         | 2850–2810 (m)<br>2720–2695 (vs)                          | Often appears as a shoulder                                                                           |
| Unsaturated C—H                                                                                                                                                              |                                                          |                                                                                                       |
| —C≡C—H                                                                                                                                                                       | 3340–3270 (w–m)                                          | Alkyl substituents at higher frequencies; unsaturated or aryl substituents at lower frequencies       |
| $\begin{array}{c} \quad \quad \text{H} \\ \quad \quad \diagup \\ \diagdown \quad \text{C}=\text{C} \\ \diagup \quad \diagdown \end{array}$                                   | 3040–2995 (m)                                            |                                                                                                       |
| $\begin{array}{c} \quad \quad \text{H} \\ \quad \quad \diagup \\ \diagdown \quad \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \quad \quad \text{H} \end{array}$           | 3095–3050 (m)<br>2990–2983 (s)                           | Asymmetric =CH <sub>2</sub> stretch<br>Symmetric =CH <sub>2</sub> stretch                             |
| $\begin{array}{c} \text{H} \quad \quad \text{R} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{H} \end{array}$     | 1419–1415 (m)<br>1309–1288 (m)                           | Plus =CH and =CH stretching bands                                                                     |
| $\begin{array}{c} \text{H} \quad \quad \text{R}_1 \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{R}_2 \end{array}$ | 1413–1399 (m)<br>909–885 (m)<br>711–684 (w)              | Plus =CH <sub>2</sub> stretching bands                                                                |



**TABLE 7.30** Raman Frequencies of Single Bonds to Hydrogen and Carbon (*Continued*)

| Group                                                                            | Band, cm <sup>-1</sup>                                                                               | Remarks                                                                                        |
|----------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------|
| Unsaturated C—H ( <i>continued</i> )                                             |                                                                                                      |                                                                                                |
|  | 1270–1251 (m)                                                                                        | Plus =CH stretching band                                                                       |
|  | 1314–1290 (m)                                                                                        | Plus =CH stretching band                                                                       |
|  | 1360–1322 (w)<br>830–800 (vw)                                                                        | Plus =CH stretching band                                                                       |
| Hydroxy O—H                                                                      |                                                                                                      |                                                                                                |
| Free —OH<br>Intermolecularly bonded<br>Aromatic —OH                              | 3650–3250 (w)<br>3400–3300 (w)<br>ca 3160 (s)                                                        |                                                                                                |
| —OH                                                                              | 1460–1320 (w)<br>1276–1205 (w–m)<br>1260 (w–m)                                                       | Common to all OH substituents<br>Primary<br>Secondary                                          |
| C—C—OH primary                                                                   | 1070–1050 (m–s)<br>1030–960 (m–s)<br>480–430 (w–m)                                                   | CCO stretching<br><br>CCO deformation                                                          |
| C—C—OH<br>Secondary<br><br>Tertiary                                              | 1135–1120 (m–s)<br>825–815 (vs)<br>500–490 (w–m)<br>1210–1200 (m–s)<br>755–730 (vs)<br>360–350 (w–m) |                                                                                                |
| —CO—O—H                                                                          | 1305–1270                                                                                            | CO stretching                                                                                  |
| N—H and C—N bonds                                                                |                                                                                                      |                                                                                                |
| Amine >N—H<br>Associated<br>Nonbonded<br>Salts<br><br>—NH <sub>2</sub>           | 3400–3250 (s)<br>3550–3250 (s)<br>2986–2974<br><br>1650–1590 (w–vs)                                  | Primary amines show two bands.<br><br>Often obscured by intense CH stretching bands<br>Bending |

**TABLE 7.30** Raman Frequencies of Single Bonds to Hydrogen and Carbon (*Continued*)

| Group                                                                          | Band, $\text{cm}^{-1}$                                                                  | Remarks                                                                                                                                                                |
|--------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| N—H and C—N Bonds ( <i>continued</i> )                                         |                                                                                         |                                                                                                                                                                        |
| Amides                                                                         |                                                                                         |                                                                                                                                                                        |
| Primary                                                                        | 3540–3500 (w)<br>3400–3380 (w)<br>1310–1250 (s)                                         | Both bands lowered ca $150\text{ cm}^{-1}$ in solid state and H bonding<br>Interaction of NH bending and CN stretching; lowered $50\text{ cm}^{-1}$ in nonbonded state |
| Secondary                                                                      | 1150–1095 (m)<br>3491–3404 (m–s)<br><br>1190–1130 (m)<br>931–865 (m–s)<br>430–395 (w–m) | Rocking of $\text{NH}_2$<br>Two bands; lowered in frequency on H bonding and in solid state                                                                            |
| —CO—N                                                                          | 607–555 (m)                                                                             | O=CN bending                                                                                                                                                           |
| $\begin{array}{c} \text{C} - \text{N} - \text{C} \\   \\ \text{C} \end{array}$ | 1070–1045 (m)                                                                           | Stretching                                                                                                                                                             |
| $\equiv\text{C}-\text{N}<$                                                     |                                                                                         |                                                                                                                                                                        |
| Primary carbon                                                                 | 1090–1060 (m)                                                                           | CN stretching                                                                                                                                                          |
| Secondary $\alpha$ carbon                                                      | 1140–1035 (m)                                                                           | Two bands but often obscured.<br>Strong band at $800\text{ cm}^{-1}$                                                                                                   |
| Tertiary $\alpha$ carbon                                                       | 1240–1020 (m)                                                                           | Two bands. Strong band also at $745\text{ cm}^{-1}$                                                                                                                    |

**TABLE 7.31** Raman Frequencies of Triple Bonds*Abbreviations Used in the Table*

m, moderately strong                      s-vs, strong to very strong  
 m-s, moderate to strong                vs, very strong  
 s, strong

| Group                                                  | Band, $\text{cm}^{-1}$                                                              | Remarks                                                                                                                                                                                                    |
|--------------------------------------------------------|-------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\text{R}-\text{C}\equiv\text{CH}$                     | 2160–2100 (vs)<br>650–600 (m)<br>356–335 (s)                                        | Monoalkyl substituted; $\text{C}\equiv\text{C}$ stretch<br>$\text{C}\equiv\text{CH}$ deformation<br>$\text{C}\equiv\text{C}-\text{C}$ bending of monoalkyls                                                |
| $\text{R}_1-\text{C}\equiv\text{C}-\text{R}_2$         | 2300–2190 (vs)                                                                      | $\text{C}\equiv\text{C}$ stretching of disubstituted alkyls; sometimes two bands                                                                                                                           |
| $-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-$      | 2264–2251 (vs)                                                                      |                                                                                                                                                                                                            |
| $-\text{C}\equiv\text{N}$                              | 2260–2240 (vs)<br>2234–2200 (vs)<br>840–800 (s-vs)<br>385–350 (m-s)<br>200–160 (vs) | Unsaturated nonaryl substituents lower the frequency and enhance the intensity.<br>Lowered ca $30\text{ cm}^{-1}$ with aryl and conjugated aliphatics<br>CCCN symmetrical stretching<br>Aliphatic nitriles |
| $\text{H}-\text{C}\equiv\text{N}$                      | 2094 (vs)                                                                           |                                                                                                                                                                                                            |
| Azides<br>$-\text{N}^+-\text{N}^-\equiv\text{N}$       | 2170–2080 (s)<br>1258–1206 (s)                                                      | Asymmetric NNN stretching<br>Symmetric NNN stretching; $\text{HN}_3$ at $1300\text{ cm}^{-1}$                                                                                                              |
| Diazonium salts<br>$\text{R}-\text{N}^+\equiv\text{N}$ | 2300–2240 (s)                                                                       |                                                                                                                                                                                                            |
| Isonitriles<br>$-\text{N}^+\equiv\text{C}^-$           | 2146–2134<br>2124–2109                                                              | Stretching of aliphatics<br>Stretching of aromatics                                                                                                                                                        |
| Thiocyanates<br>$-\text{S}-\text{C}\equiv\text{N}$     | 2260–2240 (vs)<br>650–600 (s)                                                       | Stretching of $\text{C}\equiv\text{N}$<br>Stretching of SC                                                                                                                                                 |

**TABLE 7.32** Raman Frequencies of Cumulated Double Bonds*Abbreviations Used in the Table*

s, strong

vw, very weak

vs, very strong

w, weak

| Group                                                        | Band, $\text{cm}^{-1}$                                    | Remarks                                                                                                                                                       |
|--------------------------------------------------------------|-----------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Allenes<br>$\text{C}=\text{C}=\text{C}$                      | 2000–1960 (s)<br>1080–1060 (vs)<br>356                    | Pseudo-asymmetric stretching<br>Symmetric stretching<br>$\text{C}=\text{C}=\text{C}$ bending                                                                  |
| Carbodiimides (cyanamides)<br>$-\text{N}=\text{C}=\text{N}-$ | 2140–2125 (s)<br>2150–2100 (vs)<br>1460<br>1150–1140 (vs) | Asymmetric stretching of aliphatics<br>Asymmetric stretching of aromatics; two bands<br>Symmetrical stretching of aliphatics<br>Symmetric stretching of aryls |
| Cumulenes (trienes)<br>$\text{C}=\text{C}=\text{C}=\text{C}$ | 2080–2030 (vs)<br>878                                     |                                                                                                                                                               |
| Isocyanates<br>$-\text{N}=\text{C}=\text{O}$                 | 2300–2250 (vw)<br>1450–1400 (s)                           | Asymmetric stretching<br>Symmetric stretching                                                                                                                 |
| Isothiocyanates<br>$-\text{N}=\text{C}=\text{S}$             | 2220–2100<br>690–650                                      | Two bands<br>Alkyl derivatives                                                                                                                                |
| Ketenes<br>$\text{C}=\text{C}=\text{O}$                      | 2060–2040 (vs)<br>1130 (s)<br>1374 (s)<br>1120 (s)        | Pseudo-asymmetric stretching<br>Pseudo-symmetric stretching<br>Alkyl derivatives<br>Aryl derivatives                                                          |
| Sulfinylamines<br>$\text{R}-\text{N}=\text{S}=\text{O}$      | 1306–1214 (w)<br>1155–989 (s)                             | Asymmetric stretching<br>Symmetric stretching                                                                                                                 |

TABLE 7.33 Raman Frequencies of Carbonyl Bands

Abbreviations Used in the Table

m, moderately strongs–vs, strong to very strong

m–s, moderate to strongvs, very strong

s, strongw, weak

| Group                                                                                                                | Band, cm <sup>–1</sup>                                                             | Remarks                                                                               |
|----------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| Acid anhydrides<br>—CO—O—CO—<br>Saturated<br><br>Conjugated, noncyclic                                               | 1850–1780 (m)<br>1771–1770 (m)<br>1775<br>1720                                     |                                                                                       |
| Acid fluorides —CO—F<br>Alkyl<br>Aryl                                                                                | 1840–1835<br>1812–1800                                                             |                                                                                       |
| Acid chlorides —CO—Cl<br>Alkyl<br>Aryl                                                                               | 1810–1770 (s)<br>1774<br>1731                                                      |                                                                                       |
| Acid bromides —CO—Br<br>Alkyl<br>Aryl                                                                                | 1812–1788<br>1775–1754                                                             |                                                                                       |
| Acid iodides —CO—I<br>Alkyl<br>Aryl                                                                                  | ca 1806<br>ca 1752                                                                 |                                                                                       |
| Lactones                                                                                                             | 1850–1730 (s)                                                                      |                                                                                       |
| Esters<br>Saturated<br><br>Aryl and α,β-unsaturated<br>Diesters<br>Oxalates<br>Phthalates<br>C≡C—CO—O—<br>Carbamates | 1741–1725<br><br>1727–1714<br><br>1763–1761<br>1738–1728<br>1716–1708<br>1694–1688 | Alkyl branching on carbon adjacent to C=O lowers frequency by 5–15 cm <sup>–1</sup> . |
| Aldehydes                                                                                                            | 1740–1720 (s–vs)                                                                   |                                                                                       |
| Ketones<br>Saturated<br>Aryl<br>Alicyclic<br>n = 4<br>n = 5<br>n ≥ 6                                                 | 1725–1700 (vs)<br>1700–1650 (m)<br><br>1782 (m)<br>1744 (m)<br>1725–1699 (m)       |                                                                                       |

**TABLE 7.33** Raman Frequencies of Carbonyl Bands (*Continued*)

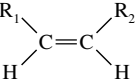
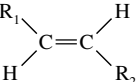
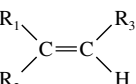
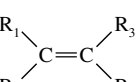
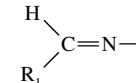
| Group                        | Band, cm <sup>-1</sup> | Remarks                                                                                                                                                            |
|------------------------------|------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Carboxylic acids             |                        |                                                                                                                                                                    |
| Mono-                        | 1686–1625 (s)          | These $\alpha$ -substituents increase the frequency:<br>F, Cl, Br, OH.<br>Solid state; often two bands<br>In solution; very broad band                             |
| Poly-                        | 1782–1645              |                                                                                                                                                                    |
|                              | 1750–1710              |                                                                                                                                                                    |
| Amino acids                  | 1743–1729              |                                                                                                                                                                    |
| Carboxylate ions             | 1690–1550 (w)          | Often masked by water deformation band near<br>1630 cm <sup>-1</sup>                                                                                               |
|                              | 1440–1340 (vs)         |                                                                                                                                                                    |
| Amino acid anion             | 1743–1729              |                                                                                                                                                                    |
|                              | 1600–1570 (w)          |                                                                                                                                                                    |
| Amides (see also Table 7.30) |                        |                                                                                                                                                                    |
| Primary                      |                        | Both <i>cis</i> and <i>trans</i> forms<br><i>Trans</i> form<br><i>Cis</i> form<br>Both <i>cis</i> and <i>trans</i> forms<br><i>Trans</i> form (no <i>cis</i> band) |
| Associated                   | 1686–1576 (m–s)        |                                                                                                                                                                    |
|                              | 1650–1620 (m)          |                                                                                                                                                                    |
| Nonbonded                    | 1715–1675 (m)          |                                                                                                                                                                    |
|                              | 1620–1585 (m)          |                                                                                                                                                                    |
| Secondary                    |                        |                                                                                                                                                                    |
| Associated                   | 1680–1630 (w)          |                                                                                                                                                                    |
|                              | 1570–1510 (w)          |                                                                                                                                                                    |
|                              | 1490–1440              |                                                                                                                                                                    |
| Nonbonded                    | 1700–1650              |                                                                                                                                                                    |
|                              | 1550–1500              |                                                                                                                                                                    |
| Tertiary                     | 1670–1630 (m)          |                                                                                                                                                                    |
| Lactams                      | 1750–1700 (m)          |                                                                                                                                                                    |

**TABLE 7.34** Raman Frequencies of Other Double Bonds*Abbreviations Used in the Table*

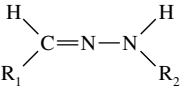
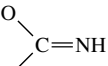
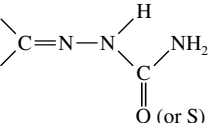
|                                |                             |
|--------------------------------|-----------------------------|
| m, moderately strong           | vs, very strong             |
| m–s, moderate to strong        | w, weak                     |
| s, strong                      | s–vs, strong to very strong |
| w–m, weak to moderately strong |                             |

| Group                                                                                                                                                                        | Band, cm <sup>-1</sup>      | Remarks                                      |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|----------------------------------------------|
| Alkenes $\text{>C=C<}$                                                                                                                                                       |                             |                                              |
| $\text{>C=C<}$                                                                                                                                                               | 1680–1576 (m–s)             | General range                                |
| $\begin{array}{c} \text{H} \quad \quad \text{R}_1 \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{H} \end{array}$   | 1648–1638 (vs)              | C=C stretching                               |
| $\begin{array}{c} \text{H} \quad \quad \text{R}_1 \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{R}_2 \end{array}$ | ca 1650 (vs)<br>270–252 (w) | C=C stretching<br>C=C–C skeletal deformation |

**TABLE 7.34** Raman Frequencies of Other Double Bonds (*Continued*)

| Group                                                                                                                                                         |                                                  | Band, cm <sup>-1</sup>                                                         |                                                                 | Remarks                                                                                     |          |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------|--------------------------------------------------------------------------------|-----------------------------------------------------------------|---------------------------------------------------------------------------------------------|----------|
| Alkenes $\text{>C=C<}$ ( <i>continued</i> )                                                                                                                   |                                                  |                                                                                |                                                                 |                                                                                             |          |
|                                                                               |                                                  | ca 1660 (vs)<br>970–952 (w)                                                    |                                                                 | C=C stretching<br>Asymmetric CC stretching                                                  |          |
|                                                                               |                                                  | 1676–1665 (s)                                                                  |                                                                 | C—C stretching                                                                              |          |
|                                                                               |                                                  | 1678–1664 (vs)<br>522–488 (w)                                                  |                                                                 | C=C stretching<br>C=C—C skeletal deformation                                                |          |
|                                                                               |                                                  | 1680–1665 (s)<br>690–678 (m–s)<br>510–485 (m)<br>424–388 (w)                   |                                                                 | C=C stretching<br>Symmetrical CC stretching<br>Skeletal deformation<br>Skeletal deformation |          |
| Haloalkene                                                                                                                                                    |                                                  | X = fluorine                                                                   | X = chlorine                                                    | X = bromine                                                                                 | X-iodine |
| $\text{>C=C<}$ stretch of haloalkanes                                                                                                                         |                                                  |                                                                                |                                                                 |                                                                                             |          |
| H <sub>2</sub> C=CHX<br>HXC=CHX<br><i>cis</i><br><i>trans</i><br>H <sub>2</sub> C=CX <sub>2</sub><br>X <sub>2</sub> C=CHX<br>X <sub>2</sub> C=CX <sub>2</sub> | 1654<br><br>1712<br>1694<br>1728<br>1792<br>1872 | 1603–1601<br><br>1590–1587<br>1578–1576<br>1616–1611<br>1589–1582<br>1577–1571 | 1596–1593<br><br>1587–1583<br>1582–1581<br>1593<br>1552<br>1547 | 1581<br><br>1543<br>1537<br><br><br><br>1465 (solid)                                        |          |
| Group                                                                                                                                                         |                                                  | Band, cm <sup>-1</sup>                                                         |                                                                 | Remarks                                                                                     |          |
| $\text{>C=N—}$ bonds                                                                                                                                          |                                                  |                                                                                |                                                                 |                                                                                             |          |
| Aldimines (azomethines)<br>                                                 |                                                  | 1673–1639<br><br>1405–1400 (s)                                                 |                                                                 | Dialkyl substituents at higher frequency; diaryl substituents at lower end of range         |          |
| Aldoximes and Ketoximes<br>$\text{>C=N—OH}$                                                                                                                   |                                                  | 1680–1617 (vs)<br>1335–1330 (w)                                                |                                                                 |                                                                                             |          |
| Azines<br>$\text{>C=N—N=C<}$                                                                                                                                  |                                                  | 1625–1608 (s)                                                                  |                                                                 |                                                                                             |          |

**TABLE 7.34** Raman Frequencies of Other Double Bonds (*Continued*)

| Group                                                                                                                      | Band, cm <sup>-1</sup>                                                                                                | Remarks                                                                                                                                  |
|----------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| $\text{>C=N—}$ bonds ( <i>continued</i> )                                                                                  |                                                                                                                       |                                                                                                                                          |
| Hydrazones<br>                             | 1660–1610 (s–vs)                                                                                                      |                                                                                                                                          |
| Imido ethers<br>                           | 1658–1648                                                                                                             | NH stretching at 3360–3327 cm <sup>-1</sup>                                                                                              |
| Semicarbazones and thio-semicarbazones<br> | 1665–1642 (vs)<br>1620–1610 (vs)                                                                                      | Aliphatic. Thiosemicarbazones fall in lower end of range. Aromatic derivatives                                                           |
| Azo compounds —N=N—                                                                                                        |                                                                                                                       |                                                                                                                                          |
| —N=N—                                                                                                                      | 1580–1570 (vs)<br>1442–1380 (vs)<br>1060–1030 (vs)                                                                    | Nonconjugated<br>Conjugated to aromatic ring<br>CN stretching in aryl compounds                                                          |
| Nitro compounds N=O                                                                                                        |                                                                                                                       |                                                                                                                                          |
| Alkyl nitrites                                                                                                             | 1660–1620 (s)                                                                                                         | N=O stretching                                                                                                                           |
| Alkyl nitrates                                                                                                             | 1635–1622 (w–m)<br>1285–1260 (vs)<br>610–562 (m)                                                                      | Asymmetric NO <sub>2</sub> stretching<br>Symmetric NO <sub>2</sub> stretching<br>NO <sub>2</sub> deformation                             |
| Nitroalkanes<br>Primary                                                                                                    | 1560–1548 (m–s)<br>1395–1370 (s)<br><br>915–898 (m–s)<br>894–873 (m–s)<br>618–609 (w)<br>640–615 (w)<br>494–472 (w–m) | Sensitive to substituents attached to CNO <sub>2</sub> group<br><br>Shoulder<br>Broad; useful to distinguish from secondary nitroalkanes |
| Secondary                                                                                                                  | 1553–1547 (m)<br>1375–1360 (s)<br>908–868 (m)<br>863–847 (s)<br>625–613 (m)<br>560–516 (s)                            | Sharp band                                                                                                                               |



**TABLE 7.34** Raman Frequencies of Other Double Bonds (*Continued*)

| Group                                                             | Band, cm <sup>-1</sup>                                                      | Remarks |
|-------------------------------------------------------------------|-----------------------------------------------------------------------------|---------|
| Nitro compounds N=O ( <i>continued</i> )                          |                                                                             |         |
| Nitroalkanes ( <i>continued</i> )<br>Tertiary                     | 1543–1533 (m)<br>1355–1345 (s)                                              |         |
| Nitrogen oxides<br>$\equiv \text{N}^+ \rightarrow \bar{\text{O}}$ | 1612–1602 (s)<br>1252 (m)<br>1049–1017 (s)<br>835 (s)<br>541 (w)<br>469 (w) |         |

**TABLE 7.35** Raman Frequencies of Aromatic Compounds*Abbreviations Used in the Table*

|                               |                                |
|-------------------------------|--------------------------------|
| m, moderately strong          | var, of variable strength      |
| m–s, moderate to strong       | vs, very strong                |
| m–vs, moderate to very strong | w, weak                        |
| s, strong                     | w–m, weak to moderately strong |
| s–vs, strong to very strong   |                                |

| Group                                     | Band, cm <sup>-1</sup>                                               | Remarks                                                                        |
|-------------------------------------------|----------------------------------------------------------------------|--------------------------------------------------------------------------------|
| Common features                           |                                                                      |                                                                                |
| Aromatic compounds                        | 3070–3020 (s)<br>1630–1570 (m–s)                                     | CH stretching<br>C—C stretching                                                |
| Substitution patterns of the benzene ring |                                                                      |                                                                                |
| Monosubstituted                           | 1180–1170 (w–m)<br>1035–1015 (s)<br>1010–990 (vs)<br><br>630–605 (w) | Characteristic feature; found also with 1,3- and 1,3,5-substitutions           |
| 1,2-Disubstituted                         | 1230–1215 (m)<br>1060–1020 (s)<br>740–715 (m)                        | Characteristic feature<br>Lowered 60 cm <sup>-1</sup> for halogen substituents |

**TABLE 7.35** Raman Frequencies of Aromatic Compounds (*Continued*)

| Group                                                          | Band, cm <sup>-1</sup>                                                 | Remarks                                                                                                                                                                      |
|----------------------------------------------------------------|------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Substitution patterns of the benzene ring ( <i>continued</i> ) |                                                                        |                                                                                                                                                                              |
| 1,3-Disubstituted                                              | 1010–990 (vs)<br>750–640 (s)                                           | Characteristic feature                                                                                                                                                       |
| 1,4-Disubstituted                                              | 1230–1200 (s–vs)<br>1180–1150 (m)<br>830–750 (vs)<br>650–630 (m–w)     | Lower frequency with Cl substituents                                                                                                                                         |
| Isolated hydrogen                                              | 1379 (s–vs)<br>1290–1200 (s)<br>745–670 (m–vs)<br>580–480 (s)          | Characteristic feature                                                                                                                                                       |
| 1,2,3-Trisubstituted                                           | 1100–1050 (m)<br>670–500 (vs)<br>490–430 (w)                           | The lighter the mass of the substituent, the higher the frequency.                                                                                                           |
| 1,2,4-Trisubstituted                                           | 750–650 (vs)<br>580–540 (var)<br>500–450 (var)                         | Lighter mass at higher frequencies                                                                                                                                           |
| 1,3,5-Trisubstituted                                           | 1010–990 (vs)                                                          |                                                                                                                                                                              |
| Completely substituted                                         | 1296 (s)<br>550 (vs)<br>450 (m)<br>361 (m)                             |                                                                                                                                                                              |
| Other aromatic compounds                                       |                                                                        |                                                                                                                                                                              |
| Naphthalenes                                                   | 1390–1370<br>1026–1012<br>767–762<br>535–512<br>519–512                | Ring breathing<br>$\alpha$ or $\beta$ substituents<br>$\beta$ substituents<br>$\alpha$ substituents<br>$\beta$ substituents                                                  |
| Disubstituted naphthalenes                                     | 773–737 (s)<br>726–705 (s)<br>690–634 (s)<br>608<br>575–569<br>544–537 | 1,2-; 1,3-; 2,3-; 2,6-; 2,7-<br>1,3-; 1,4-(two bands); 1,6-; 1,7-(two bands)<br>1,2-; 1,4-(two bands); 1,5-; 1,8-(two bands)<br>1,3-<br>1,2-; 1,3-; 1,6-<br>1,2-; 1,7-; 1,8- |
| Anthracenes                                                    | 1415–1385                                                              | Ring breathing                                                                                                                                                               |

TABLE 7.36 Raman Frequencies of Sulfur Compounds

Abbreviations Used in the Table

m, moderately strongs–vs, strong to very strong

m–s, moderate to strongvs, very strong

s, strongw–m, weak to moderately strong

| Group                                                                                                                                                                        | Band, cm <sup>−1</sup>                                                  | Remarks                                                                                                                                                     |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| —S—H                                                                                                                                                                         | 2590–2560 (s)                                                           | SH stretching for both aliphatic and aromatic                                                                                                               |
| ≧C=S                                                                                                                                                                         | 1065–1050 (m)<br>735–690 (vs)                                           | Solid state                                                                                                                                                 |
| ≧S=O<br>In (RO <sub>2</sub> ) <sub>2</sub> SO<br>In (R <sub>2</sub> N) <sub>2</sub> SO<br>In R <sub>2</sub> SO<br>SOF <sub>2</sub><br>SOCl <sub>2</sub><br>SOBr <sub>2</sub> | 1209–1198<br>1108<br>1070–1010 (w–m)<br>1308<br>1233<br>1121            | One or two bands<br><br>Broad                                                                                                                               |
| —SO <sub>2</sub> —                                                                                                                                                           | 1330–1260 (m–s)<br>1155–1110 (s)<br>610–540 (m)<br>512–485 (m)          | Asymmetric SO <sub>2</sub> stretching<br>Symmetric SO <sub>2</sub> stretching<br>Scissoring mode of aryls<br>Scissoring mode of alkyls                      |
| —SO <sub>2</sub> —N<                                                                                                                                                         | ca 1322 (m)<br>1163–1138 (s)<br>524–510 (s)                             | Asymmetric SO <sub>2</sub> stretching<br>Symmetric SO <sub>2</sub> stretching<br>Scissoring mode                                                            |
| —SO <sub>2</sub> —O                                                                                                                                                          | 1363–1338 (w–m)<br><br>1192–1165 (vs)<br>589–517 (w–m)                  | SO <sub>2</sub> stretching. Aryl substituents occur at higher range.<br><br>Scissoring (two bands). Aryl substituents occur at higher range of frequencies. |
| —SO <sub>2</sub> —S—                                                                                                                                                         | 1334–1305 (m–s)<br>1128–1126 (s)<br>559–553 (m–s)                       |                                                                                                                                                             |
| X—SO <sub>2</sub> —X                                                                                                                                                         | 1412–1361 (w–m)<br>(F) (Cl)<br>1263–1168 (s)<br>(F) (Cl)<br>596–531 (s) |                                                                                                                                                             |
| —O—SO <sub>2</sub> —O—                                                                                                                                                       | 1388–1372 (s)<br>1196–1188 (vs)                                         |                                                                                                                                                             |
| —O—C—S—<br>  <br>S                                                                                                                                                           | 670–620 (vs)<br>480–450 (vs)                                            | C=S stretching<br>CS stretching                                                                                                                             |
| ≧C—SH                                                                                                                                                                        | 920 (m)<br>850–820 (m)                                                  | C—SH deformation of aryls                                                                                                                                   |

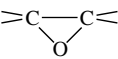
**TABLE 7.36** Raman Frequencies of Sulfur Compounds (*Continued*)

| Group                                                                                                                                            | Band, cm <sup>-1</sup>                                                                                   | Remarks                                                                                                                                                                                 |
|--------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\equiv\text{C}-\text{S}-$                                                                                                                       | 752 (vs), 731 (vs)<br>742–722 (m–s)<br>698 (w), 678 (s)<br>693–639 (s)<br>651–610 (s–vs)<br>589–585 (vs) | With vinyl group attached<br>With CH <sub>3</sub> attached<br>With allyl group attached<br>Ethyl or longer alkyl chain<br>Isopropyl group attached<br><i>tert</i> -Butyl group attached |
| $(\text{CH}_2)_n \text{S}$<br>$n = 2$<br>$n = 4$<br>$n = 5$                                                                                      | 1112<br>688<br>659                                                                                       |                                                                                                                                                                                         |
| $\equiv\text{C}-(\text{S}-\text{S})_n-\text{C}\equiv$<br><br>Didi- <i>n</i> -alkyl disulfides<br>Di- <i>tert</i> -butyl disulfide<br>Trisulfides | 715–620 (vs)<br>525–510 (vs)<br>576 (s)<br>543 (m)<br>510–480 (s)                                        | Two bands; CS stretching<br>Two bands; SS stretching<br>CS stretching<br>SS stretching<br>SS stretching                                                                                 |

**TABLE 7.37** Raman Frequencies of Ethers*Abbreviations Used in the Table*

m, moderately strong  
s, strong

var, of variable strength  
vs, very strong

| Group                                                                              | Band, cm <sup>-1</sup>                                      | Remarks                                                                                                                                                              |
|------------------------------------------------------------------------------------|-------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\equiv\text{C}-\text{O}-\text{C}\equiv$<br>Aliphatic                              | 1200–1070 (m)<br><br>930–830 (s)<br>800–700 (s)<br>550–400  | Asymmetrical COC stretching. Symmetrical substitution gives higher frequencies<br>Symmetrical COC stretching<br>Bracing at $\alpha$ carbon gives higher frequencies. |
| Aromatic                                                                           | 1310–1210 (m)<br>1050–1010 (m)                              |                                                                                                                                                                      |
| $\equiv\text{C}-\text{O}-\text{C}(\text{O})-\text{O}-\text{C}\equiv$               | 1145–1129 (m)<br><br>900–800 (vs)<br>537–370 (s)<br>396–295 |                                                                                                                                                                      |
|  | 1280–1240 (s)                                               | Ring breathing                                                                                                                                                       |
| $-\text{O}-\text{O}-$                                                              | 800–770 (var)                                               |                                                                                                                                                                      |

**TABLE 7.37** Raman Frequencies of Ethers (*Continued*)

| Group                                                       | Band, $\text{cm}^{-1}$                      | Remarks |
|-------------------------------------------------------------|---------------------------------------------|---------|
| $(\text{CH}_2)_n \text{O}$<br>$n = 3$<br>$n = 4$<br>$n = 5$ | 1040–1010 (s)<br>920–900 (s)<br>820–800 (s) |         |

**TABLE 7.38** Raman Frequencies of Halogen Compounds*Abbreviations Used in the Table*

m–s, moderate to strong      var, of variable strength  
 s, strong                              vs, very strong

| Group                                    | Band, $\text{cm}^{-1}$                                      | Remarks                                                                                                                 |
|------------------------------------------|-------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------|
| C—F                                      | 1400–870                                                    | Correlations of limited applicability because of vibrational coupling with stretching                                   |
| C—Cl<br>Primary<br>Secondary<br>Tertiary | 350–290 (s)<br>660–650 (vs)<br>760–605 (s)<br>620–540 (var) | CCl bending; general<br><br>May be one to four bands<br>May be one to three bands                                       |
| =C—Cl                                    | 844–564<br>438–396<br>381–170                               |                                                                                                                         |
| =CCl <sub>2</sub>                        | 601–441<br>300–235                                          |                                                                                                                         |
| C—Br                                     | 690–490 (s)<br>305–258 (m–s)                                | Often several bands; primary at higher range of frequencies. Tertiary has very strong band at ca 520 $\text{cm}^{-1}$ . |
| =C—Br                                    | 745–565<br>356–318<br>240–115                               |                                                                                                                         |
| =CBr <sub>2</sub>                        | 467–265<br>185–145                                          |                                                                                                                         |
| C—I                                      | 663–595<br>309<br>154–85                                    |                                                                                                                         |
| =C—I                                     | ca 180                                                      | Solid state                                                                                                             |
| =CI <sub>2</sub>                         | ca 265<br>ca 105                                            | Solid state<br>Solid state                                                                                              |

**TABLE 7.39** Raman Frequencies of Miscellaneous Compounds*Abbreviations Used in the Table*

m, moderately strong

vs, very strong

s, strong

vvs, very very strong

| Group              | Band, $\text{cm}^{-1}$ | Remarks          |
|--------------------|------------------------|------------------|
| C—As               | 570–550 (vs)           | CAs stretching   |
|                    | 240–220 (vs)           | CAsC deformation |
| C—Pb               | 480–420 (s)            | CPb stretching   |
| C—Hg               | 570–510 (vvs)          | CHg stretching   |
| C—Si               | 1300–1200 (s)          | CSi stretching   |
| C—Sn               | 600–450 (s)            | CSn stretching   |
| P—H                | 2350–2240 (m)          | PH stretching    |
| Heterocyclic rings |                        |                  |
| Trimethylene oxide | 1029                   | 2-Substituted    |
| Trimethylene imine | 1026                   |                  |
| Tetrahydrofuran    | 914                    |                  |
| Pyrrolidine        | 899                    |                  |
| 1,3-Dioxolane      | 939                    |                  |
| 1,4-Dioxane        | 834                    |                  |
| Piperidine         | 815                    |                  |
| Tetrahydropyran    | 818                    |                  |
| Morpholine         | 832                    |                  |
| Piperazine         | 836                    |                  |
| Furan              | 1515–1460              |                  |
|                    | 1140                   |                  |
| Pyrazole           | 1040–990               |                  |
| Pyrrole            | 1420–1360 (vs)         |                  |
|                    | 1144                   |                  |
| Thiophene          | 1410 (s)               |                  |
|                    | 1365 (s)               |                  |
|                    | 1085 (vs)              |                  |
|                    | 1035 (s)               |                  |
|                    | 832 (vs)               |                  |
|                    | 610 (s)                |                  |
| Pyridine           | 1030 (vs)              |                  |
|                    | 990 (vs)               |                  |

**TABLE 7.40** Principal Argon-Ion Laser Plasma Lines

| Wavelength, nm | Wavenumber, cm <sup>-1</sup> | Relative intensity | Shift relative to<br>488.0 nm, cm <sup>-1</sup> | Shift relative to<br>514.5 nm,<br>cm <sup>-1</sup> |
|----------------|------------------------------|--------------------|-------------------------------------------------|----------------------------------------------------|
| 487.9860       | 20 486.67                    | 5000               | 0                                               |                                                    |
| 488.9033       | 20 448.23                    | 200                | 38.4                                            |                                                    |
| 490.4753       | 20 382.70                    | 130                | 104.0                                           |                                                    |
| 493.3206       | 20 265.13                    | 970                | 221.5                                           |                                                    |
| 496.5073       | 20 135.07                    | 960                | 351.6                                           |                                                    |
| 497.2157       | 20 106.39                    | 330                | 380.3                                           |                                                    |
| 500.9334       | 19 957.16                    | 1500               | 529.5                                           |                                                    |
| 501.7160       | 19 926.03                    | 620                | 560.6                                           |                                                    |
| 506.2036       | 19 749.39                    | 1400               | 737.3                                           |                                                    |
| 514.1790       | 19 443.06                    | 360                | 1043.6                                          |                                                    |
| 514.5319       | 19 429.73                    | 1000               | 1056.9                                          | 0                                                  |
| 516.5774       | 19 352.79                    | 38                 | 1133.9                                          | 76.9                                               |
| 517.6233       | 19 313.69                    | 41                 | 1173.0                                          | 116.0                                              |
| 521.6816       | 19 163.44                    | 20                 | 1323.2                                          | 266.3                                              |
| 528.6895       | 18 909.43                    | 150                | 1577.2                                          | 520.3                                              |
| 539.7522       | 18 521.87                    | 18                 | 1964.8                                          | 907.9                                              |
| 545.4307       | 18 329.04                    | 19                 | 2157.6                                          | 1100.7                                             |
| 555.8703       | 17 984.81                    | 30                 | 2501.9                                          | 1444.9                                             |
| 560.6734       | 17 830.75                    | 48                 | 2655.9                                          | 1599.0                                             |
| 565.0705       | 17 692.00                    | 29                 | 2794.7                                          | 1737.7                                             |
| 565.4450       | 17 680.28                    | 27                 | 2806.4                                          | 1749.4                                             |
| 569.1650       | 17 564.73                    | 27                 | 2921.9                                          | 1865.0                                             |
| 577.2326       | 17 319.24                    | 69                 | 3167.4                                          | 2110.5                                             |
| 581.2746       | 17 198.80                    | 49                 | 3287.9                                          | 2230.9                                             |
| 598.5920       | 16 701.24                    | 23                 | 3785.4                                          | 2728.5                                             |
| 610.3546       | 16 379.38                    | 91                 | 4107.3                                          | 3050.4                                             |
| 611.4929       | 16 348.90                    | 1750               | 4137.8                                          | 3080.8                                             |
| 612.3368       | 16 326.36                    | 100                | 4160.3                                          | 3103.4                                             |
| 613.8660       | 16 285.69                    | 97                 | 4201.0                                          | 3144.0                                             |
| 617.2290       | 16 196.96                    | 1400               | 4289.7                                          | 3232.8                                             |
| 624.3125       | 16 013.19                    | 590                | 4473.5                                          | 3416.5                                             |
| 639.9215       | 15 622.60                    | 160                | 4864.1                                          | 3807.1                                             |
| 641.6308       | 15 580.98                    | 50                 | 4905.7                                          | 3848.8                                             |

## 7.7 NUCLEAR MAGNETIC RESONANCE

**TABLE 7.41** Nuclear Properties of the Elements

In the following table the magnetic moment  $\mu$  is in multiples of the nuclear magneton  $\mu_N(eh/4\pi mc)$  with diamagnetic correction. The spin  $I$  is in multiples of  $h/2\pi$ , and the electric quadrupole moment  $Q$  is in multiples of  $10^{-28}$  square meters. Nuclei with spin  $\frac{1}{2}$  have no quadrupole moment. Sensitivity is for equal numbers of nuclei at constant field. NMR frequency at any magnetic field is the entry for column 5 multiplied by the value of the magnetic field in kilogauss. For example, in a magnetic field of 23.490 kG, protons will process at 4.2576  $\times$  23.490 kG = 100.0 MHz. Radionuclides are denoted with an asterisk.

The data were extracted from M. Lederer and V. S. Shirley, *Table of Isotopes*, 7th ed., Wiley-Interscience, New York, 1978; A. H. Wapstra and G. Audi, "The 1983 Atomic Mass Evaluation," *Nucl. Phys. A* **432**:1–54 (1985); V. S. Shirley, ed., *Table of Radioactive Isotopes*, 8th ed., Wiley-Interscience, New York, 1986; and P. Raghavan, "Table of Nuclear Moments," *At. Data Nucl. Data Tables*, **42**:189 (1989).

| Nuclide          | Natural abundance, % | Spin $I$      | Sensitivity at constant field relative to $^1\text{H}$ | NMR frequency for a 1-kG field, MHz | Magnetic moment $\mu/\mu_N$ , $\text{J} \cdot \text{T}^{-1}$ | Electric quadrupole moment $Q$ , $10^{-28} \text{ m}^2$ |
|------------------|----------------------|---------------|--------------------------------------------------------|-------------------------------------|--------------------------------------------------------------|---------------------------------------------------------|
| $^1\text{n}$     | *                    | $\frac{1}{2}$ | 0.321 39                                               | 2.916 39                            | −1.913 043                                                   |                                                         |
| $^1\text{H}$     | 99.985               | $\frac{1}{2}$ | 1.000 00                                               | 4.257 64                            | 2.792 847                                                    |                                                         |
| $^2\text{H}$     | 0.015                | 1             | 0.009 65                                               | 0.653 57                            | 0.857 438                                                    | 0.002 860                                               |
| $^3\text{H}$     | *                    | $\frac{1}{2}$ | 1.213 54                                               | 4.541 37                            | 2.978 963                                                    |                                                         |
| $^3\text{He}$    | 0.0001               | $\frac{1}{2}$ | 0.442 12                                               | 3.243 52                            | −2.127 624                                                   |                                                         |
| $^6\text{Li}$    | 7.5                  | 1             | 0.008 50                                               | 0.626 60                            | 0.822 047                                                    | 0.000 82                                                |
| $^7\text{Li}$    | 92.5                 | $\frac{3}{2}$ | 0.293 55                                               | 1.654 78                            | 3.256 427                                                    | −0.040 1                                                |
| $^9\text{Be}$    | 100                  | $\frac{3}{2}$ | 0.013 89                                               | 0.598 6                             | −1.177 9                                                     | 0.052 88                                                |
| $^{10}\text{B}$  | 19.9                 | 3             | 0.019 85                                               | 0.457 51                            | 1.800 645                                                    | 0.084 59                                                |
| $^{11}\text{B}$  | 80.1                 | $\frac{3}{2}$ | 0.165 22                                               | 1.366 26                            | 2.688 649                                                    | 0.040 59                                                |
| $^{13}\text{C}$  | 1.10                 | $\frac{1}{2}$ | 0.015 91                                               | 1.070 81                            | 0.702 412                                                    |                                                         |
| $^{14}\text{N}$  | 99.634               | 1             | 0.001 01                                               | 0.307 76                            | 0.403 761                                                    | 0.020 2                                                 |
| $^{15}\text{N}$  | 0.366                | $\frac{1}{2}$ | 0.001 04                                               | 0.431 72                            | −0.283 189                                                   |                                                         |
| $^{17}\text{O}$  | 0.038                | $\frac{5}{2}$ | 0.029 10                                               | 0.577 41                            | −1.893 80                                                    | −0.025 58                                               |
| $^{19}\text{F}$  | 100                  | $\frac{1}{2}$ | 0.834 00                                               | 4.007 65                            | 2.628 867                                                    |                                                         |
| $^{21}\text{Ne}$ | 0.27                 | $\frac{3}{2}$ | 0.002 46                                               | 0.336 30                            | −0.661 797                                                   | 0.101 55                                                |
| $^{22}\text{Na}$ | *                    | 3             | 0.018 1                                                | 0.443 4                             | 1.745                                                        |                                                         |
| $^{23}\text{Na}$ | 100                  | $\frac{3}{2}$ | 0.092 70                                               | 1.126 86                            | 2.217 522                                                    | 0.108 9                                                 |
| $^{25}\text{Mg}$ | 10.00                | $\frac{5}{2}$ | 0.002 68                                               | 0.260 82                            | −0.855 46                                                    | 0.199 4                                                 |
| $^{27}\text{Al}$ | 100                  | $\frac{5}{2}$ | 0.206 89                                               | 1.110 28                            | 3.641 504                                                    | 0.140 3                                                 |
| $^{29}\text{Si}$ | 4.67                 | $\frac{1}{2}$ | 0.007 86                                               | 0.846 53                            | −0.555 29                                                    |                                                         |
| $^{31}\text{P}$  | 100                  | $\frac{1}{2}$ | 0.066 52                                               | 1.725 10                            | 1.131 60                                                     |                                                         |
| $^{33}\text{S}$  | 0.75                 | $\frac{3}{2}$ | 0.002 27                                               | 0.327 16                            | 0.643 821                                                    | −0.067 8                                                |
| $^{35}\text{S}$  | *                    | $\frac{3}{2}$ | 0.008 50                                               | 0.508                               | 1.00                                                         | 0.045                                                   |
| $^{35}\text{Cl}$ | 75.77                | $\frac{3}{2}$ | 0.004 72                                               | 0.417 64                            | 0.821 874                                                    | −0.081 65                                               |
| $^{36}\text{Cl}$ | *                    | 2             | 0.012 1                                                | 0.489 3                             | 1.283 8                                                      | −0.016 8                                                |
| $^{37}\text{Cl}$ | 24.23                | $\frac{3}{2}$ | 0.002 72                                               | 0.347 64                            | 0.684 124                                                    | −0.064 35                                               |
| $^{37}\text{Ar}$ | *                    | $\frac{3}{2}$ | 0.012 76                                               | 0.581 8                             | 1.145                                                        |                                                         |
| $^{39}\text{K}$  | 93.258               | $\frac{3}{2}$ | 0.000 51                                               | 0.198 93                            | 0.391 466                                                    | 0.060 1                                                 |
| $^{40}\text{K}$  | 0.0117               | 4             | 0.005 23                                               | 0.247 37                            | −1.298 099                                                   | −0.074 9                                                |
| $^{41}\text{K}$  | 6.730                | $\frac{3}{2}$ | 0.000 084                                              | 0.109 19                            | 0.214 870                                                    | 0.073 3                                                 |
| $^{43}\text{Ca}$ | 0.135                | $\frac{7}{2}$ | 0.006 42                                               | 0.286 88                            | −1.317 26                                                    | −0.0408                                                 |
| $^{45}\text{Sc}$ | 100                  | $\frac{7}{2}$ | 0.302 44                                               | 1.035 88                            | 4.756 483                                                    | −0.22                                                   |
| $^{47}\text{Ti}$ | 7.3                  | $\frac{5}{2}$ | 0.002 10                                               | 0.240 40                            | −0.788 48                                                    | 0.29                                                    |
| $^{49}\text{Ti}$ | 5.5                  | $\frac{7}{2}$ | 0.003 78                                               | 0.240 47                            | −1.104 17                                                    | 0.24                                                    |
| $^{50}\text{V}$  | 0.250                | 6             | 0.055 71                                               | 0.425 04                            | 3.345 689                                                    | 0.21                                                    |



TABLE 7.41 Nuclear Properties of the Elements (Continued)

| Nuclide           | Natural abundance, % | Spin <i>I</i> | Sensitivity at constant field relative to <sup>1</sup> H | NMR frequency for a 1-kG field, MHz | Magnetic moment $\mu/\mu_N$ , J · T <sup>-1</sup> | Electric quadrupole moment <i>Q</i> , 10 <sup>-28</sup> m <sup>2</sup> |
|-------------------|----------------------|---------------|----------------------------------------------------------|-------------------------------------|---------------------------------------------------|------------------------------------------------------------------------|
| <sup>51</sup> V   | 99.750               | ½             | 0.383 60                                                 | 1.121 30                            | 5.148 706                                         | −0.052                                                                 |
| <sup>53</sup> Cr  | 9.501                | ¾             | 0.000 91                                                 | 0.241 14                            | −0.474 54                                         | −0.15                                                                  |
| <sup>55</sup> Mn  | 100                  | ½             | 0.178 81                                                 | 1.057 60                            | 3.468 72                                          | 0.33                                                                   |
| <sup>57</sup> Fe  | 2.1                  | ½             | 0.000 03                                                 | 0.138 15                            | 0.090 623                                         |                                                                        |
| <sup>59</sup> Co  | 100                  | ¾             | 0.278 41                                                 | 1.007 7                             | 4.627                                             | 0.42                                                                   |
| <sup>61</sup> Ni  | 1.140                | ¾             | 0.003 59                                                 | 0.381 13                            | −0.750 02                                         | 0.162                                                                  |
| <sup>63</sup> Cu  | 69.17                | ¾             | 0.093 42                                                 | 1.129 79                            | 2.223 29                                          | −0.220                                                                 |
| <sup>65</sup> Cu  | 30.83                | ¾             | 0.114 84                                                 | 1.210 27                            | 2.381 67                                          | −0.204                                                                 |
| <sup>67</sup> Zn  | 4.1                  | ½             | 0.002 87                                                 | 0.266 93                            | 0.875 479                                         | 0.150                                                                  |
| <sup>69</sup> Ga  | 60.108               | ¾             | 0.069 71                                                 | 1.024 75                            | 2.016 59                                          | 0.170                                                                  |
| <sup>71</sup> Ga  | 39.892               | ¾             | 0.143 00                                                 | 1.302 04                            | 2.562 27                                          | 0.100                                                                  |
| <sup>73</sup> Ge  | 7.73                 | ¾             | 0.001 41                                                 | 0.148 97                            | −0.879 468                                        | −0.173                                                                 |
| <sup>75</sup> As  | 100                  | ¾             | 0.025 36                                                 | 0.731 48                            | 1.439 475                                         | 0.314                                                                  |
| <sup>77</sup> Se  | 7.63                 | ½             | 0.007 03                                                 | 0.815 66                            | 0.535 042                                         |                                                                        |
| <sup>79</sup> Br  | 50.69                | ¾             | 0.079 45                                                 | 1.070 39                            | 2.106 399                                         | 0.331                                                                  |
| <sup>81</sup> Br  | 49.31                | ¾             | 0.099 51                                                 | 1.153 81                            | 2.270 562                                         | 0.276                                                                  |
| <sup>83</sup> Kr  | 11.5                 | ¾             | 0.001 90                                                 | 0.164 42                            | −0.970 669                                        | 0.253                                                                  |
| <sup>85</sup> Rb  | 72.165               | ½             | 0.010 61                                                 | 0.412 53                            | 1.353 03                                          | 0.274                                                                  |
| <sup>87</sup> Rb  | 27.835               | ¾             | 0.177 03                                                 | 1.398 07                            | 2.751 24                                          | 0.132                                                                  |
| <sup>87</sup> Sr  | 7.00                 | ¾             | 0.002 72                                                 | 0.185 24                            | −1.093 603                                        | 0.335                                                                  |
| <sup>89</sup> Y   | 100                  | ½             | 0.000 12                                                 | 0.209 49                            | −0.137 415                                        |                                                                        |
| <sup>91</sup> Zr  | 11.22                | ½             | 0.009 49                                                 | 0.397 47                            | −1.303 62                                         | −0.206                                                                 |
| <sup>93</sup> Nb  | 100                  | ¾             | 0.488 21                                                 | 1.045 20                            | 6.170 5                                           | −0.32                                                                  |
| <sup>95</sup> Mo  | 15.92                | ¾             | 0.003 27                                                 | 0.278 74                            | −0.914 2                                          | −0.022                                                                 |
| <sup>97</sup> Mo  | 9.55                 | ¾             | 0.003 49                                                 | 0.284 62                            | −0.933 5                                          | −0.255                                                                 |
| <sup>99</sup> Tc  | *                    | ¾             | 0.381 74                                                 | 0.963                               | 5.684 7                                           | −0.129                                                                 |
| <sup>99</sup> Ru  | 12.7                 | ½             | 0.001 13                                                 | 0.195 53                            | −0.641 3                                          | 0.079                                                                  |
| <sup>101</sup> Ru | 17.0                 | ½             | 0.001 59                                                 | 0.219 2                             | −0.718 8                                          | 0.457                                                                  |
| <sup>103</sup> Rh | 100                  | ½             | 0.000 03                                                 | 0.134 76                            | −0.088 40                                         |                                                                        |
| <sup>105</sup> Pd | 22.33                | ¾             | 0.001 13                                                 | 0.195 7                             | −0.642                                            | 0.660                                                                  |
| <sup>107</sup> Ag | 51.839               | ½             | 0.000 066 9                                              | 0.173 30                            | −0.113 680                                        |                                                                        |
| <sup>109</sup> Ag | 48.161               | ½             | 0.000 101                                                | 0.199 24                            | −0.130 691                                        |                                                                        |
| <sup>111</sup> Cd | 12.80                | ½             | 0.009 66                                                 | 0.906 89                            | −0.594 886                                        |                                                                        |
| <sup>113</sup> Cd | 12.22                | ½             | 0.011 06                                                 | 0.948 68                            | −0.622 301                                        |                                                                        |
| <sup>113</sup> In | 4.3                  | ¾             | 0.351 21                                                 | 0.936 52                            | 5.528 9                                           | 0.799                                                                  |
| <sup>115</sup> In | 95.7                 | ¾             | 0.353 48                                                 | 0.938 54                            | 5.540 8                                           | 0.81                                                                   |
| <sup>115</sup> Sn | 0.34                 | ½             | 0.035 61                                                 | 1.400 74                            | −9.18 84                                          |                                                                        |
| <sup>117</sup> Sn | 7.68                 | ½             | 0.046 05                                                 | 1.526 06                            | −1.001 05                                         |                                                                        |
| <sup>119</sup> Sn | 8.59                 | ½             | 0.052 73                                                 | 1.596 56                            | −1.047 28                                         |                                                                        |
| <sup>121</sup> Sb | 57.36                | ¾             | 0.163 02                                                 | 1.025 49                            | 3.363 4                                           | −0.36                                                                  |
| <sup>123</sup> Sb | 42.64                | ¾             | 0.046 59                                                 | 0.555 30                            | 2.549 8                                           | −0.49                                                                  |
| <sup>123</sup> Te | 0.908                | ½             | 0.018 37                                                 | 1.123 46                            | −0.736 948                                        |                                                                        |
| <sup>125</sup> Te | 7.139                | ½             | 0.032 20                                                 | 1.354 51                            | −0.888 505                                        |                                                                        |
| <sup>127</sup> I  | 100                  | ¾             | 0.095 40                                                 | 0.857 76                            | 2.813 327                                         | −0.789                                                                 |
| <sup>129</sup> Xe | 26.4                 | ½             | 0.021 62                                                 | 1.186 01                            | −0.777 976                                        |                                                                        |
| <sup>131</sup> Xe | 21.2                 | ¾             | 0.002 82                                                 | 0.351 58                            | 0.691 862                                         | −0.12                                                                  |
| <sup>133</sup> Cs | 100                  | ¾             | 0.048 38                                                 | 0.562 32                            | 2.582 025                                         | −0.003 7                                                               |
| <sup>135</sup> Ba | 6.592                | ¾             | 0.005 00                                                 | 0.425 81                            | 0.837 943                                         | 0.160                                                                  |
| <sup>137</sup> Ba | 11.23                | ¾             | 0.006 97                                                 | 0.476 33                            | 0.937 365                                         | 0.245                                                                  |
| <sup>138</sup> La | * 0.0902             | 5             | 0.094 04                                                 | 0.566 14                            | 3.713 646                                         | 0.45                                                                   |

**TABLE 7.41** Nuclear Properties of the Elements (*Continued*)

| Nuclide           | Natural abundance, % | Spin $I$      | Sensitivity at constant field relative to $^1\text{H}$ | NMR frequency for a 1-kG field, MHz | Magnetic moment $\mu/\mu_N$ , $\text{J} \cdot \text{T}^{-1}$ | Electric quadrupole moment $Q$ , $10^{-28} \text{ m}^2$ |
|-------------------|----------------------|---------------|--------------------------------------------------------|-------------------------------------|--------------------------------------------------------------|---------------------------------------------------------|
| $^{139}\text{La}$ | 99.9098              | $\frac{7}{2}$ | 0.060 58                                               | 0.606 10                            | 2.783 045                                                    | 0.20                                                    |
| $^{137}\text{Ce}$ | *                    | $\frac{3}{2}$ | 0.006 41                                               | 0.462                               | 0.91                                                         |                                                         |
| $^{139}\text{Ce}$ | *                    | $\frac{3}{2}$ | 0.006 41                                               | 0.462                               | 0.91                                                         |                                                         |
| $^{141}\text{Ce}$ | *                    | $\frac{7}{2}$ | 0.003 64                                               | 0.237                               | 1.09                                                         |                                                         |
| $^{141}\text{Pr}$ | 100                  | $\frac{5}{2}$ | 0.334 83                                               | 1.303 55                            | 4.275 4                                                      | -0.059                                                  |
| $^{143}\text{Nd}$ | 12.18                | $\frac{7}{2}$ | 0.003 39                                               | 0.231 9                             | -1.065                                                       | -0.63                                                   |
| $^{145}\text{Nd}$ | 8.30                 | $\frac{7}{2}$ | 0.000 79                                               | 0.142 9                             | -0.656                                                       | -0.33                                                   |
| $^{143}\text{Pm}$ | *                    | $\frac{5}{2}$ | 0.235 10                                               | 1.16                                | 3.8                                                          |                                                         |
| $^{147}\text{Pm}$ | *                    | $\frac{7}{2}$ | 0.049 40                                               | 0.57                                | 2.6                                                          | 0.70                                                    |
| $^{147}\text{Sm}$ | 15.0                 | $\frac{7}{2}$ | 0.001 52                                               | 0.177 47                            | -0.814 9                                                     | -0.26                                                   |
| $^{149}\text{Sm}$ | 13.8                 | $\frac{7}{2}$ | 0.000 85                                               | 0.146 31                            | -0.671 8                                                     | 0.094                                                   |
| $^{151}\text{Eu}$ | 47.8                 | $\frac{5}{2}$ | 0.179 29                                               | 1.058 54                            | 3.471 8                                                      | 0.903                                                   |
| $^{153}\text{Eu}$ | 52.2                 | $\frac{5}{2}$ | 0.015 44                                               | 0.467 44                            | 1.533 1                                                      | 2.41                                                    |
| $^{155}\text{Gd}$ | 14.80                | $\frac{3}{2}$ | 0.000 15                                               | 0.131 7                             | -0.259 1                                                     | 1.27                                                    |
| $^{157}\text{Gd}$ | 15.65                | $\frac{3}{2}$ | 0.000 33                                               | 0.1727                              | -0.339 9                                                     | 1.35                                                    |
| $^{159}\text{Tb}$ | 100                  | $\frac{3}{2}$ | 0.069 45                                               | 1.023                               | 2.014                                                        | 1.432                                                   |
| $^{161}\text{Dy}$ | 18.9                 | $\frac{5}{2}$ | 0.000 48                                               | 1.465 3                             | -0.480 6                                                     | 2.47                                                    |
| $^{163}\text{Dy}$ | 24.9                 | $\frac{5}{2}$ | 0.001 30                                               | 0.205 07                            | 0.672 6                                                      | 2.65                                                    |
| $^{165}\text{Ho}$ | 100                  | $\frac{7}{2}$ | 0.204 23                                               | 0.908 81                            | 4.173                                                        | 3.58                                                    |
| $^{167}\text{Er}$ | 22.95                | $\frac{7}{2}$ | 0.000 507                                              | 0.122 81                            | -0.563 9                                                     | 3.57                                                    |
| $^{169}\text{Tm}$ | 100                  | $\frac{1}{2}$ | 0.000 566                                              | 3.531                               | -0.231 6                                                     |                                                         |
| $^{171}\text{Yb}$ | 14.3                 | $\frac{1}{2}$ | 0.005 52                                               | 0.752 59                            | 0.493 67                                                     |                                                         |
| $^{173}\text{Yb}$ | 16.12                | $\frac{5}{2}$ | 0.001 35                                               | 0.207 301                           | -0.679 89                                                    | 2.80                                                    |
| $^{175}\text{Lu}$ | 97.41                | $\frac{7}{2}$ | 0.031 28                                               | 0.486 24                            | 2.232 7                                                      | 3.49                                                    |
| $^{176}\text{Lu}$ | * 2.59               | 7             | 0.039 75                                               | 0.345 1                             | 3.169                                                        | 4.97                                                    |
| $^{177}\text{Hf}$ | 18.606               | $\frac{7}{2}$ | 0.001 40                                               | 0.172 81                            | 0.793 5                                                      | 3.36                                                    |
| $^{179}\text{Hf}$ | 13.629               | $\frac{9}{2}$ | 0.000 55                                               | 0.108 56                            | -0.640 9                                                     | 3.79                                                    |
| $^{180}\text{Ta}$ | 0.012                | 9             | 0.102 51                                               | 0.404                               | 4.77                                                         |                                                         |
| $^{181}\text{Ta}$ | 99.988               | $\frac{7}{2}$ | 0.037 44                                               | 0.516 25                            | 2.3705                                                       | 3.17                                                    |
| $^{183}\text{W}$  | 14.3                 | $\frac{1}{2}$ | 0.000 08                                               | 0.179 56                            | 0.117 785                                                    |                                                         |
| $^{185}\text{Re}$ | 37.40                | $\frac{5}{2}$ | 0.138 70                                               | 0.971 7                             | 3.1871                                                       | 2.18                                                    |
| $^{187}\text{Re}$ | * 62.60              | $\frac{5}{2}$ | 0.143 00                                               | 0.981 7                             | 3.219 7                                                      | 2.07                                                    |
| $^{187}\text{Os}$ | 1.6                  | $\frac{1}{2}$ | 0.000 01                                               | 0.098 56                            | 0.064 652                                                    |                                                         |
| $^{189}\text{Os}$ | 16.1                 | $\frac{3}{2}$ | 0.002 44                                               | 0.335 35                            | 0.659 933                                                    | 0.856                                                   |
| $^{191}\text{Ir}$ | 37.3                 | $\frac{3}{2}$ | 0.000 03                                               | 0.076 6                             | 0.150 7                                                      | 0.816                                                   |
| $^{193}\text{Ir}$ | 62.7                 | $\frac{3}{2}$ | 0.000 04                                               | 0.0832                              | 0.163 7                                                      | 0.751                                                   |
| $^{195}\text{Pt}$ | 33.8                 | $\frac{1}{2}$ | 0.010 39                                               | 0.929 20                            | 0.609 52                                                     |                                                         |
| $^{197}\text{Au}$ | 100                  | $\frac{3}{2}$ | 0.000 03                                               | 0.074 06                            | 0.145 746                                                    | 0.547                                                   |
| $^{199}\text{Hg}$ | 16.87                | $\frac{1}{2}$ | 0.005 94                                               | 0.771 21                            | 0.505 885                                                    |                                                         |
| $^{201}\text{Hg}$ | 13.18                | $\frac{3}{2}$ | 0.001 49                                               | 0.284 68                            | -0.560 226                                                   | 0.386                                                   |
| $^{203}\text{Tl}$ | 29.524               | $\frac{1}{2}$ | 0.195 981                                              | 2.473 10                            | 1.622 258                                                    |                                                         |
| $^{205}\text{Tl}$ | 70.476               | $\frac{1}{2}$ | 0.201 82                                               | 2.497 42                            | 1.638 215                                                    |                                                         |
| $^{207}\text{Pb}$ | 22.1                 | $\frac{1}{2}$ | 0.009 55                                               | 0.903 38                            | 0.592 58                                                     |                                                         |
| $^{209}\text{Bi}$ | 100                  | $\frac{9}{2}$ | 0.144 33                                               | 0.696 28                            | 4.110 6                                                      | -0.50                                                   |
| $^{229}\text{Th}$ | *                    | $\frac{5}{2}$ | 0.000 42                                               | 0.140                               | 0.46                                                         | 4.30                                                    |
| $^{231}\text{Pa}$ | *                    | $\frac{3}{2}$ | 0.069 03                                               | 1.02                                | 2.01                                                         | -1.72                                                   |
| $^{235}\text{U}$  | * 0.7200             | $\frac{7}{2}$ | 0.000 15                                               | 0.083                               | -0.38                                                        | 4.936                                                   |
| $^{237}\text{Np}$ | *                    | $\frac{5}{2}$ | 0.132 64                                               | 0.957                               | 3.14                                                         | 3.886                                                   |
| $^{239}\text{Pu}$ | *                    | $\frac{1}{2}$ | 0.000 38                                               | 0.309                               | 0.203                                                        |                                                         |
| $^{243}\text{Am}$ | *                    | $\frac{5}{2}$ | 0.017 88                                               | 0.491                               | 1.61                                                         | 4.21                                                    |

**TABLE 7.42** Proton Chemical Shifts

Values are given on the officially approved  $\delta$  scale;  $\tau = 10.00 - \delta$ .

*Abbreviations Used in the Table*

R, alkyl group      Ar, aryl group

| Substituent group                         | Methyl protons | Methylene protons | Methine proton |
|-------------------------------------------|----------------|-------------------|----------------|
| HC—C—CH <sub>2</sub>                      | 0.95           | 1.20              | 1.55           |
| HC—C—NR <sub>2</sub>                      | 1.05           | 1.45              | 1.70           |
| HC—C—C=C                                  | 1.00           | 1.35              | 1.70           |
| HC—C—C=O                                  | 1.05           | 1.55              | 1.95           |
| HC—C—NRAr                                 | 1.10           | 1.50              | 1.80           |
| HC—C—H(C=O)R                              | 1.10           | 1.50              | 1.90           |
| HC—C—(C=O)NR <sub>2</sub>                 | 1.10           | 1.50              | 1.80           |
| HC—C—(C=O)Ar                              | 1.15           | 1.55              | 1.90           |
| HC—C—(C=O)OR                              | 1.15           | 1.70              | 1.90           |
| HC—C—Ar                                   | 1.15           | 1.55              | 1.80           |
| HC—C—OH                                   | 1.20           | 1.50              | 1.75           |
| HC—C—OR                                   | 1.20           | 1.50              | 1.75           |
| HC—C—C≡CR                                 | 1.20           | 1.50              | 1.80           |
| HC—C—C≡N                                  | 1.25           | 1.65              | 2.00           |
| HC—C—SR                                   | 1.25           | 1.60              | 1.90           |
| HC—C—OAr                                  | 1.30           | 1.55              | 2.00           |
| HC—C—O(C=O)R                              | 1.30           | 1.60              | 1.80           |
| HC—C—SH                                   | 1.30           | 1.60              | 1.65           |
| HC—C—(S=O)R<br>and HC—C—SO <sub>2</sub> R | 1.35           | 1.70              |                |
| HC—C—NR <sub>3</sub> <sup>+</sup>         | 1.40           | 1.75              | 2.05           |
| HC—C—O—N=O                                | 1.40           |                   |                |
| HC—C—O(C=O)CF <sub>3</sub>                | 1.40           | 1.65              |                |
| HC—C—CL                                   | 1.55           | 1.80              | 1.95           |
| HC—C—F                                    | 1.55           | 1.85              | 2.15           |
| HC—C—NO <sub>2</sub>                      | 1.60           | 2.05              | 2.50           |
| HC—C—O(C=O)Ar                             | 1.65           | 1.75              | 1.85           |
| HC—C—I                                    | 1.75           | 1.80              | 2.10           |
| HC—C—Br                                   | 1.80           | 1.85              | 1.90           |
| HC—CH <sub>2</sub>                        | 0.90           | 1.30              | 1.50           |
| HC—C=C                                    | 1.60           | 2.05              |                |
| HC—C≡C                                    | 1.70           | 2.20              | 2.80           |
| HC—(C=O)OR                                | 2.00           | 2.25              | 2.50           |
| HC—(C=O)NR <sub>2</sub>                   | 2.00           | 2.25              | 2.40           |
| HC—SR                                     | 2.05           | 2.55              | 3.00           |
| HC—O—O                                    | 2.10           | 2.30              | 2.55           |
| HC—(C=O)R                                 | 2.10           | 2.35              | 2.65           |
| HC—C≡N                                    | 2.15           | 2.45              | 2.90           |
| HC—I                                      | 2.15           | 3.15              | 4.25           |
| HC—CHO                                    | 2.20           | 2.40              |                |
| HC—Ar                                     | 2.25           | 2.45              | 2.85           |
| HC—NR <sub>2</sub>                        | 2.25           | 2.40              | 2.80           |
| HC—SSR                                    | 2.35           | 2.70              |                |
| HC—(C=O)Ar                                | 2.40           | 2.70              | 3.40           |
| HC—SAr                                    | 2.40           |                   |                |
| HC—NRAr                                   | 2.60           | 3.10              | 3.60           |
| HC—SO <sub>2</sub> R and HC—(SO)R         | 2.60           | 3.05              |                |
| HC—Br                                     | 2.70           | 3.40              | 4.10           |
| HC—NR <sub>3</sub> <sup>+</sup>           | 2.95           | 3.10              | 3.60           |

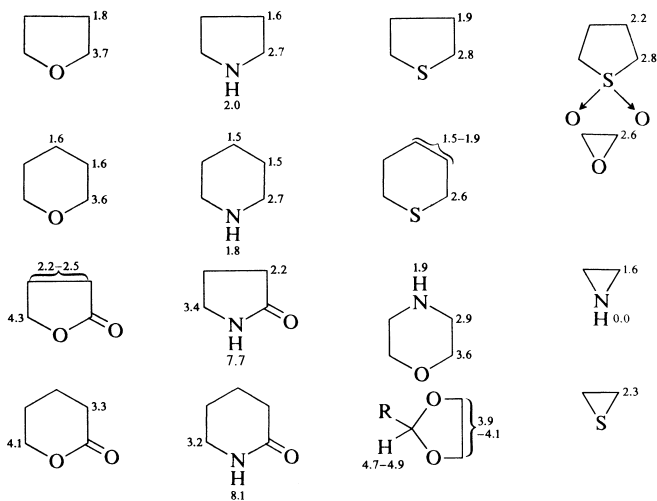
**TABLE 7.42** Proton Chemical Shifts (*Continued*)

| Substituent group        | Methyl protons | Methylene protons | Methine proton |
|--------------------------|----------------|-------------------|----------------|
| HC—NH(C=O)R              | 2.95           | 3.35              | 3.85           |
| HC—SO <sub>3</sub> R     | 2.95           |                   |                |
| HC—Cl                    | 3.05           | 3.45              | 4.05           |
| HC—OH and HC—OR          | 3.20           | 3.40              | 3.60           |
| HC—PAR <sub>3</sub>      | 3.20           | 3.40              |                |
| HC—NH <sub>2</sub>       | 3.50           | 3.75              | 4.05           |
| HC—O(C=O)R               | 3.65           | 4.10              | 4.95           |
| HC—OAr                   | 3.80           | 4.00              | 4.60           |
| HC—O(C=O)Ar              | 3.80           | 4.20              | 5.05           |
| HC—O(C=O)CF <sub>1</sub> | 3.95           | 4.30              |                |
| HC—F                     | 4.25           | 4.50              | 4.80           |
| HC—NO <sub>2</sub>       | 4.30           | 4.35              | 4.60           |
| Cyclopropane             |                | 0.20              | 0.40           |
| Cyclobutane              |                | 2.45              |                |
| Cyclopentane             |                | 1.65              |                |
| Cyclohexane              |                | 1.50              | 1.80           |
| Cycloheptane             |                | 1.25              |                |

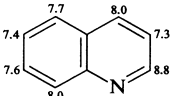
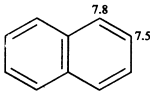
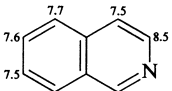
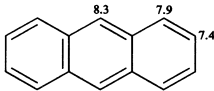
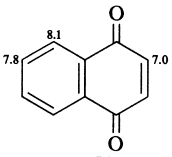
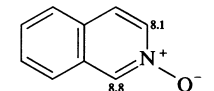
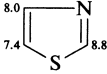
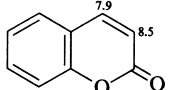
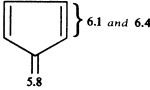
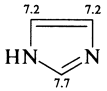
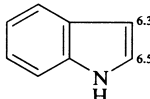
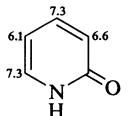
  

| Substituent group | Proton shift | Substituent group  | Proton shift |
|-------------------|--------------|--------------------|--------------|
| HC≡CH             | 2.35         | HO—C=O             | 10–12        |
| HC≡CAr            | 2.90         | HO—SO <sub>2</sub> | 11–12        |
| HC≡C—C=C          | 2.75         | HO—Ar              | 4.5–6.5      |
| HAr               | 7.20         | HO—R               | 0.5–4.5      |
| HCO—O             | 8.1          | HS—Ar              | 2.8–3.6      |
| HCO—R             | 9.4–10.0     | HS—R               | 1–2          |
| HCO—Ar            | 9.7–10.5     | HN—Ar              | 3–6          |
| HO—N=C (oxime)    | 9–12         | HN—R               | 0.5–5        |

## Saturated heterocyclic ring systems



**TABLE 7.42** Proton Chemical Shifts (*Continued*)

| Unsaturated cyclic systems                                                        |                                                                                   |                                                                                   |                                                                                   |  |  |
|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|--|--|
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |

**TABLE 7.43** Estimation of Chemical Shift for Protons of —CH<sub>2</sub>— and Methine Groups

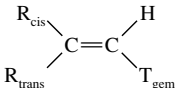
$$\delta_{\text{CH}_2} = 0.23 + C_1 + C_2 \quad \delta_{\text{CH}} = 0.23 + C_1 + C_2 + C_3$$

| X*                 | C   | X*      | C   | X*     | C   |
|--------------------|-----|---------|-----|--------|-----|
| —CH <sub>3</sub>   | 0.5 | —SR     | 1.6 | —OR    | 2.4 |
| —CF <sub>3</sub>   | 1.1 | —C≡C—Ar | 1.7 | —Cl    | 2.5 |
| >C=C<              | 1.3 | —CN     | 1.7 | —OH    | 2.6 |
| —C≡C—R             | 1.4 | —CO—R   | 1.7 | —N=C=S | 2.9 |
| —COOR              | 1.5 | —I      | 1.8 | —OCOR  | 3.1 |
| —NR <sub>2</sub>   | 1.6 | —Ph     | 1.8 | —OPh   | 3.2 |
| —CONR <sub>2</sub> | 1.6 | —Br     | 2.3 |        |     |

\* R, alkyl group; Ar, aryl group; Ph, phenyl group.

**TABLE 7.44** Estimation of Chemical Shift for Proton Attached to a Double Bond

Positive Z values indicate a downfield shift, and an arrow indicates the point of attachment of the substituent group to the double bond.

$$\delta_{\text{C}=\text{C}-\text{H}} = 5.25 - Z_{\text{gem}} + Z_{\text{cis}} + Z_{\text{trans}}$$


| R                                                                                                      | $Z_{\text{gem}}$ , ppm | $Z_{\text{cis}}$ , ppm | $Z_{\text{trans}}$ , ppm |
|--------------------------------------------------------------------------------------------------------|------------------------|------------------------|--------------------------|
| →H                                                                                                     | 0                      | 0                      | 0                        |
| →alkyl                                                                                                 | 0.45                   | -0.22                  | -0.28                    |
| →alkyl—ring (5- or 6-member)                                                                           | 0.69                   | -0.25                  | -0.28                    |
| →CH <sub>2</sub> O—                                                                                    | 0.64                   | -0.01                  | -0.02                    |
| →CH <sub>2</sub> S—                                                                                    | 0.71                   | -0.13                  | -0.22                    |
| →CH <sub>2</sub> X (X: F, Cl, Br)                                                                      | 0.70                   | 0.11                   | -0.04                    |
| →CH <sub>2</sub> N<                                                                                    | 0.58                   | -0.10                  | -0.08                    |
|  C=C (isolated)        | 1.00                   | -0.09                  | -0.23                    |
|  C=C (conjugated)      | 1.24                   | 0.02                   | -0.05                    |
| →C≡N                                                                                                   | 0.27                   | 0.75                   | 0.55                     |
| →C≡C—                                                                                                  | 0.47                   | 0.38                   | 0.12                     |
|  C=O (isolated)        | 1.10                   | 1.12                   | 0.87                     |
|  C=O (conjugated)      | 1.06                   | 0.91                   | 0.74                     |
| →COOH (isolated)                                                                                       | 0.97                   | 1.41                   | 0.71                     |
| →COOH (conjugated)                                                                                     | 0.80                   | 0.98                   | 0.32                     |
| →COOR (isolated)                                                                                       | 0.80                   | 1.18                   | 0.55                     |
| →COOR (conjugated)                                                                                     | 0.78                   | 1.01                   | 0.46                     |
|  C=O                  | 1.02                   | 0.95                   | 1.17                     |
|  C=O                 | 1.37                   | 0.98                   | 0.46                     |
|  C=O                 | 1.11                   | 1.46                   | 1.01                     |
| →OR (R: aliphatic)                                                                                     | 1.22                   | -1.07                  | -1.21                    |
| →OR (R: conjugated)                                                                                    | 1.21                   | -0.60                  | -1.00                    |
| →OCOR                                                                                                  | 2.11                   | -0.35                  | -0.64                    |
| →CH <sub>2</sub> —C=O; →CH <sub>2</sub> —C≡N                                                           | 0.69                   | -0.08                  | -0.06                    |
| →CH <sub>2</sub> —aromatic ring                                                                        | 1.05                   | -0.29                  | -0.32                    |
| →F                                                                                                     | 1.54                   | -0.40                  | -1.02                    |
| →Cl                                                                                                    | 1.08                   | 0.18                   | 0.13                     |
| →Br                                                                                                    | 1.07                   | 0.45                   | 0.55                     |
| →I                                                                                                     | 1.14                   | 0.81                   | 0.88                     |
| →N—R (R: aliphatic)                                                                                    | 0.80                   | -1.26                  | -1.21                    |
|  N—R (R: conjugated) | 1.17                   | -0.53                  | -0.99                    |

**TABLE 7.44** Estimation of Chemical Shift for Proton Attached to a Double Bond (*Continued*)

| R                                                                                      | $Z_{\text{gem}}$ , ppm | $Z_{\text{cis}}$ , ppm | $Z_{\text{trans}}$ , ppm |
|----------------------------------------------------------------------------------------|------------------------|------------------------|--------------------------|
| $\begin{array}{c}   \quad   \\ \rightarrow \text{N} - \text{C} = \text{O} \end{array}$ | 2.08                   | −0.57                  | −0.72                    |
| →aromatic                                                                              | 1.38                   | 0.36                   | −0.07                    |
| →CF <sub>3</sub>                                                                       | 0.66                   | 0.61                   | 0.32                     |
| →aromatic ( <i>o</i> -substituted)                                                     | 1.65                   | 0.19                   | 0.09                     |
| →SR                                                                                    | 1.11                   | −0.29                  | −0.13                    |
| →SO <sub>2</sub>                                                                       | 1.55                   | 1.16                   | 0.93                     |

**TABLE 7.45** Chemical Shifts in Monosubstituted Benzene

$$\delta = 7.27 + \Delta_i$$

| Substituent                       | $\Delta_{\text{ortho}}$ | $\Delta_{\text{meta}}$ | $\Delta_{\text{para}}$ |
|-----------------------------------|-------------------------|------------------------|------------------------|
| NO <sub>2</sub>                   | 0.94                    | 0.18                   | 0.39                   |
| CHO                               | 0.58                    | 0.20                   | 0.26                   |
| COOH                              | 0.80                    | 0.16                   | 0.25                   |
| COOCH <sub>3</sub>                | 0.71                    | 0.08                   | 0.20                   |
| COCl                              | 0.82                    | 0.21                   | 0.35                   |
| CCl <sub>3</sub>                  | 0.8                     | 0.2                    | 0.2                    |
| COCH <sub>3</sub>                 | 0.62                    | 0.10                   | 0.25                   |
| CN                                | 0.26                    | 0.18                   | 0.30                   |
| CONH <sub>2</sub>                 | 0.65                    | 0.20                   | 0.22                   |
| NH <sub>3</sub> <sup>+</sup>      | 0.4                     | 0.2                    | 0.2                    |
| CH <sub>2</sub> X*                | 0.0–0.1                 | 0.0–0.1                | 0.0–0.1                |
| CH <sub>3</sub>                   | −0.16                   | −0.09                  | −0.17                  |
| CH <sub>2</sub> CH <sub>3</sub>   | −0.15                   | −0.06                  | −0.18                  |
| CH(CH <sub>3</sub> ) <sub>2</sub> | −0.14                   | −0.09                  | −0.18                  |
| C(CH <sub>3</sub> ) <sub>2</sub>  | −0.09                   | 0.05                   | −0.23                  |
| F                                 | −0.30                   | −0.02                  | −0.23                  |
| Cl                                | 0.01                    | −0.06                  | −0.08                  |
| Br                                | 0.19                    | −0.12                  | −0.05                  |
| I                                 | 0.39                    | −0.25                  | −0.02                  |
| NH <sub>2</sub>                   | −0.76                   | −0.25                  | −0.63                  |
| OCH <sub>3</sub>                  | −0.46                   | −0.10                  | −0.41                  |
| OH                                | −0.49                   | −0.13                  | −0.2                   |
| OCOR                              | −0.2                    | 0.1                    | −0.2                   |
| NHCH <sub>3</sub>                 | −0.8                    | −0.3                   | −0.6                   |
| N(CH <sub>3</sub> ) <sub>2</sub>  | −0.60                   | −0.10                  | −0.62                  |

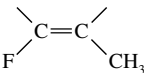
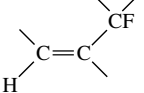
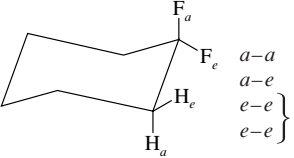
\* X = Cl, alkyl, OH, or NH<sub>2</sub>.

TABLE 7.46 Proton Spin Coupling Constants

| Structure | <i>J</i> , Hz | Structure    | <i>J</i> , Hz                                                                    |
|-----------|---------------|--------------|----------------------------------------------------------------------------------|
|           | 12–15         |              | 2–3<br>3–4<br>2–4<br>2–5<br>5–6<br>3.5–5.0<br>1.5<br>3.4                         |
|           | 6–8           |              | <i>o</i><br><i>m</i><br><i>p</i><br>6–12<br>4–8<br>1.5–2.5                       |
|           | 5             |              | <i>o</i><br><i>m</i><br><i>p</i><br>2.5<br>1.5<br>0                              |
|           | 4–8           |              | <i>a-a</i><br><i>a-e</i><br><i>e-e</i><br>8–10<br>2–3<br>2–3                     |
|           | 6–8           | Cyclopentane | <i>cis</i><br><i>trans</i><br>4–6<br>4–6                                         |
|           | 1–3           | Cyclobutane  | <i>cis</i><br><i>trans</i><br>8<br>8                                             |
|           | 8–16          | Cyclopropane | <i>cis</i><br><i>trans</i><br><i>gem</i><br>9–11<br>6–8<br>4–6                   |
|           | 0–3           |              | <i>o</i><br><i>m</i><br><i>p</i><br>6–10<br>1–3<br>0–1                           |
|           | 6–14          |              | 1–2<br>2–3<br>8–9<br>6                                                           |
|           | 11–18         |              | 2–3<br>3–4<br>2–4<br>3–5<br>2–5<br>2–6<br>5–6<br>7–9<br>1–2<br>1–2<br>0–1<br>0–1 |
|           | 0.5–3         |              | 1–2<br>1–3<br>2–3<br>2–3<br>3–4<br>1–2<br>1–3                                    |
|           | 0.5–3         |              | 45–52                                                                            |
|           | 4–10          |              | <i>gauche</i><br><i>trans</i><br>0–12<br>10–45                                   |
|           | 10–13         |              | <i>gem</i><br><i>cis</i><br><i>trans</i><br>72–90<br>–3 to 20<br>12–40           |
|           | 6             |              |                                                                                  |
|           | 0–3           |              |                                                                                  |
|           | 0–3           |              |                                                                                  |
|           | 0–2           |              |                                                                                  |
|           | 2–4           |              |                                                                                  |
|           | 5–7           |              |                                                                                  |
|           | 6–9           |              |                                                                                  |
|           | 10–13         |              |                                                                                  |
|           | 4–5           |              |                                                                                  |
|           | 3             |              |                                                                                  |
|           | 5–6           |              |                                                                                  |
|           | 0             |              |                                                                                  |
|           | 7             |              |                                                                                  |
|           | 6             |              |                                                                                  |
|           | 2             |              |                                                                                  |
|           | 6             |              |                                                                                  |
|           | 4             |              |                                                                                  |
|           | 1.8           |              |                                                                                  |
|           | 3.5           |              |                                                                                  |
|           | 0–1           |              |                                                                                  |
|           | 1–2           |              |                                                                                  |



**TABLE 7.46** Proton Spin Coupling Constants (*Continued*)

| Structure                                                                        | $J$ , Hz | Structure                                                                         | $J$ , Hz           |
|----------------------------------------------------------------------------------|----------|-----------------------------------------------------------------------------------|--------------------|
|  | 2–4      |  | 21                 |
|  | 0–6      |  | 34<br>12<br>$<5-8$ |

**TABLE 7.47** Proton Chemical Shifts of Reference Compounds*Relative to tetramethylsilane.*

| Compound                  | $\delta$ , ppm | Solvent(s)                           |
|---------------------------|----------------|--------------------------------------|
| Sodium acetate            | 1.90           | D <sub>2</sub> O                     |
| 1,2-Dibromoethane         | 3.63           | CDCl <sub>3</sub>                    |
| 1,1,2,2-Tetrachloroethane | 5.95           | CDCl <sub>3</sub> ; CCl <sub>4</sub> |
| 1,4-Benzoquinone          | 6.78           | CDCl <sub>3</sub> ; CCl <sub>4</sub> |
| 1,4-Dichlorobenzene       | 7.23           | CCl <sub>4</sub>                     |
| 1,3,5-Trinitrobenzene     | 9.21           | DMSO- $d_6$ *                        |
|                           | 9.55           | CHCl <sub>3</sub>                    |

\* DMSO, dimethyl sulfoxide.

**TABLE 7.48** Solvent Positions of Residual Protons in Incompletely Deuterated Solvents*Relative to tetramethylsilane.*

| Solvent                                                         | Group          | $\delta$ , ppm |
|-----------------------------------------------------------------|----------------|----------------|
| Acetic- $d_3$ acid- $d_1$                                       | Methyl         | 2.05           |
|                                                                 | Hydroxyl       | 11.5*          |
| Acetone- $d_6$                                                  | Methyl         | 2.057          |
| Acetonitrile- $d_3$                                             | Methyl         | 1.95           |
| Benzene- $d_6$                                                  | Methine        | 6.78           |
| <i>tert</i> -Butanol- $d_1$ (CH <sub>3</sub> ) <sub>3</sub> COD | Methyl         | 1.28           |
| Chloroform- $d_1$                                               | Methine        | 7.25           |
| Cyclohexane- $d_{12}$                                           | Methylene      | 1.40           |
| Deuterium oxide                                                 | Hydroxyl       | 4.7*           |
| Dimethyl- $d_6$ -formamide- $d_1$                               | Methyl         | 2.75; 2.95     |
|                                                                 | Formyl         | 8.05           |
| Dimethyl- $d_6$ sulfoxide                                       | Methyl         | 2.51           |
|                                                                 | Absorbed water | 3.3*           |
| 1,4-Dioxane- $d_8$                                              | Methylene      | 3.55           |
| Hexamethyl- $d_{18}$ -phosphoramidate                           | Methyl         | 2.60           |
| Methanol- $d_4$                                                 | Methyl         | 3.35           |
|                                                                 | Hydroxyl       | 4.8*           |
| Dichloromethane- $d_2$                                          | Methylene      | 5.35           |

\* These values may vary greatly, depending upon the solute and its concentration.

**TABLE 7.48** Solvent Positions of Residual Protons in Incompletely Deuterated Solvents (*Continued*)

| Solvent                     | Group       | $\delta$ , ppm |
|-----------------------------|-------------|----------------|
| Pyridine- $d_5$             | C-2 Methine | 8.5            |
|                             | C-3 Methine | 7.0            |
|                             | C-4 Methine | 7.35           |
| Toluene- $d_8$              | Methyl      | 2.3            |
|                             | Methine     | 7.2            |
| Trifluoroacetic acid- $d_1$ | Hydroxyl    | 11.3*          |

\* These values may vary greatly, depending upon the solute and its concentration.

**TABLE 7.49** Carbon-13 Chemical Shifts

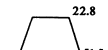
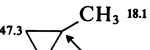
Values given in ppm on the  $\delta$  scale, relative to tetramethylsilane.

| Substituent group                           | Primary carbon | Secondary carbon            | Tertiary carbon | Quaternary carbon |
|---------------------------------------------|----------------|-----------------------------|-----------------|-------------------|
| <i>Alkanes</i>                              |                |                             |                 |                   |
| C—C                                         | 5–30           | 25–45                       | 23–58           | 28–50             |
| C—O                                         | 45–60          | 42–71                       | 62–78           | 73–86             |
| C—N                                         | 13–45          | 44–58                       | 50–70           | 60–75             |
| C—S                                         | 10–30          | 22–42                       | 55–67           | 53–62             |
| C—halide (I to Cl)                          | 3–25           | 3–40                        | 34–58           | 35–75             |
| Substituent group                           | $\delta$ , ppm | Substituent group           |                 | $\delta$ , ppm    |
| Cyclopropane                                | –5–5           | Aromatics:                  |                 |                   |
| Cycloalkane C <sub>4</sub> –C <sub>10</sub> | 5–25           | Aryl-C                      |                 | 125–145           |
| Mercaptanes                                 | 5–70           | Aryl-P                      |                 | 119–128           |
| Amines:                                     |                | Aryl-N                      |                 | 128–138           |
| R <sub>2</sub> N—C                          | 20–70          | Aryl-O                      |                 | 133–152           |
| Aryl—N                                      | 128–138        | Azomethines                 |                 | 145–162           |
| Sulfoxides, sulfones                        | 35–55          | Carbonates                  |                 | 159–162           |
| Alcohols R—OH                               | 45–87          | Ureas                       |                 | 150–170           |
| Ethers R—O—R                                | 57–87          | Anhydrides                  |                 | 150–175           |
| Nitro R—NO <sub>2</sub>                     | 60–78          | Amides                      |                 | 154–178           |
| Alkynes:                                    |                | Oximes                      |                 | 155–165           |
| HC≡CR                                       | 63–73          | Esters:                     |                 |                   |
| RC≡CR                                       | 72–95          | Saturated                   |                 | 158–165           |
| Acetals, ketals                             | 88–112         | $\alpha,\beta$ -Unsaturated |                 | 165–176           |
| Thiocyanates R—SCN                          | 96–118         | Isocyanides R—NC            |                 | 162–175           |
| Alkenes:                                    |                | Carboxylic acids:           |                 |                   |
| H <sub>2</sub> C=                           | 100–122        | Nonconjugated               |                 | 162–165           |
| R <sub>2</sub> C=                           | 110–150        | Conjugated                  |                 | 165–184           |
| Heteroaromatics:                            |                | Salts (anion)               |                 | 175–195           |
| C=N                                         | 100–152        | Ketones:                    |                 |                   |
| C <sub><math>\alpha</math></sub>            | 142–160        | $\alpha$ -Halo              |                 | 160–200           |
| Cyanates R—OCN                              | 105–120        | Nonconjugated               |                 | 192–202           |
| Isocyanates R—NCO                           | 115–135        | $\alpha,\beta$ -Unsaturated |                 | 202–220           |
| Isothiocyanates R—NCS                       | 115–142        | Imides                      |                 | 165–180           |
| Nitriles, cyanides                          | 117–124        | Acyl chlorides R—CO—Cl      |                 | 165–183           |

**TABLE 7.49** Carbon-13 Chemical Shifts (*Continued*)

| Substituent group | $\delta$ , ppm | Substituent group       | $\delta$ , ppm |
|-------------------|----------------|-------------------------|----------------|
| Thioureas         | 165–185        | Thioketones $R-C(=S)-R$ | 190–202        |
| Aldehydes:        |                | Carbonyl $M(CO)_n$      | 190–218        |
| $\alpha$ -Halo    | 170–190        | Allenes $=C=C=$         | 197–205        |
| Nonconjugated     | 182–192        |                         |                |
| Conjugated        | 192–208        |                         |                |

## Saturated heterocyclic ring systems

|                                                                                   |                  |                                                                                   |                  |                                                                                   |                  |                                                                                   |                  |
|-----------------------------------------------------------------------------------|------------------|-----------------------------------------------------------------------------------|------------------|-----------------------------------------------------------------------------------|------------------|-----------------------------------------------------------------------------------|------------------|
|  | 39.5             |  | 18.7             |  | 18.2             |  | 22.9, 72.6       |
|  | 29.7, 27.5       |  | 26.0, 68.0       |  | 31.2, 31.7       |  | 25.7, 47.1       |
|  | 24.9, 27.7, 69.5 |  | 26.6, 27.8, 29.1 |  | 25.9, 27.8, 47.9 |  | 66.5             |
|  | 92.8, 65.9, 26.6 |  | 22.8, 51.5       |  | 24.4, 56.7, 48.0 |  | 47.3, 18.1, 47.6 |

## Unsaturated cyclic systems

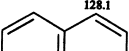
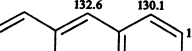
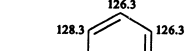
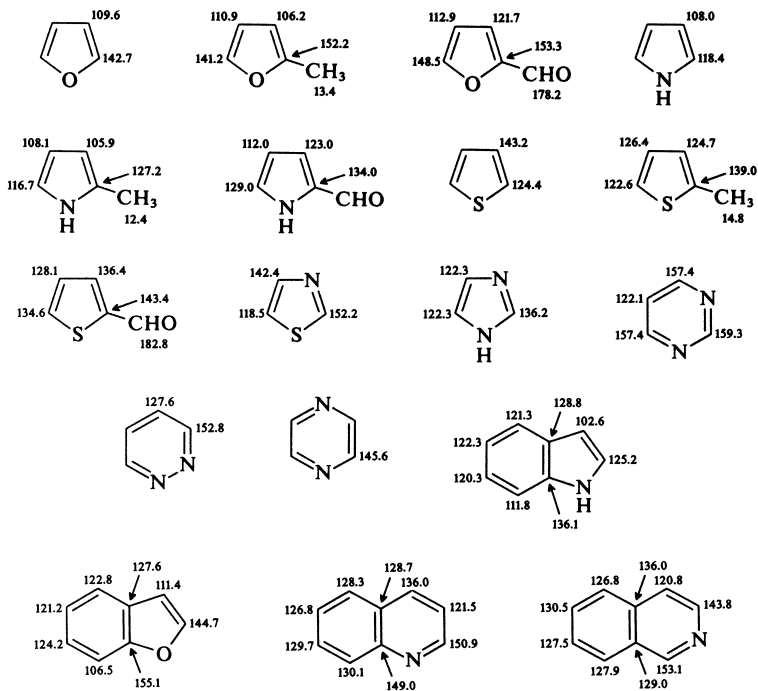
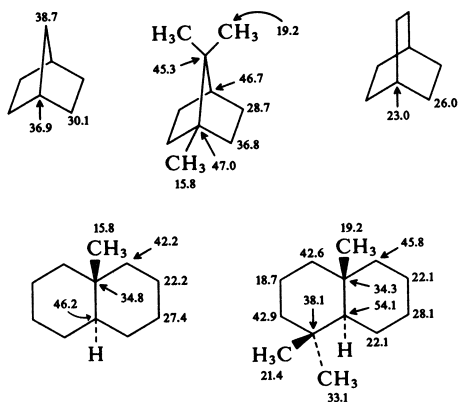
|                                                                                     |                            |                                                                                     |                                          |                                                                                     |                     |                                                                                   |                                |
|-------------------------------------------------------------------------------------|----------------------------|-------------------------------------------------------------------------------------|------------------------------------------|-------------------------------------------------------------------------------------|---------------------|-----------------------------------------------------------------------------------|--------------------------------|
|    | 30.2, 137.2                |    | 130.8, 32.6, 22.1                        |    | 127.3, 24.5, 22.1   |  | 107.1, 149.7, 36.2, 28.9, 26.9 |
|  | 165.1, 133.8               |  | 150.7, 129.3                             |  | 128.1, 125.9, 133.7 |                                                                                   |                                |
|  | 132.6, 130.1, 125.5, 132.2 |  | 126.3, 126.3, 122.2, 131.9, 126.6, 130.1 |                                                                                     |                     |                                                                                   |                                |

TABLE 7.49 Carbon-13 Chemical Shifts (*Continued*)Unsaturated cyclic systems (*continued*)

## Saturated alicyclic ring systems



**TABLE 7.50** Estimation of Chemical Shifts of Alkane Carbons  
*Relative to tetramethylsilane.*

Positive terms indicate a downfield shift.

$$\delta_C = -2.6 + 9.1n_\alpha + 9.4n_\beta - 2.5n_\gamma + 0.3n_\delta + 0.1n_\epsilon \quad (\text{plus any correction factors})$$

where  $n_\alpha$  is the number of carbons bonded directly to the  $i$ th carbon atom and  $n_\beta$ ,  $n_\gamma$ ,  $n_\delta$ , and  $n_\epsilon$  are the number of carbon atoms two, three, four, and five bonds removed. The constant is the chemical shift for methane.

| Chain branching* | Correction factor | Chain branching* | Correction factor |
|------------------|-------------------|------------------|-------------------|
| 1°(3°)           | − 1.1             | 4°(1°)           | − 1.5             |
| 1°(4°)           | − 3.4             | 2°(4°)           | − 7.2             |
| 2°(3°)           | − 2.5             | 3°(3°)           | − 9.5             |
| 3°(2°)           | − 3.7             | 4°(2°)           | − 8.4             |

\* 1° signifies a CH<sub>3</sub>— group; 2°, a —CH<sub>2</sub>— group; 3°, a >CH— group; and 4°, a >C< group. 1° (3°) signifies a methyl group bound to a >CH— group, and so on.

**Examples:** For 3-methylpentane, CH<sub>3</sub>—CH<sub>2</sub>—CH(CH<sub>3</sub>)—CH<sub>2</sub>—CH<sub>3</sub>,

$$\delta_{C=2} = -2.6 + 9.1(2) + 9.4(2) - 2.5 - 1(1)[2^\circ(3^\circ)] = 29.4$$

$$\delta_{C=3} = -2.6 + 9.1(3) + 9.4(2) + (2)[3^\circ(2^\circ)] = 36.2$$

**TABLE 7.51** Effect of Substituent Groups on Alkyl Chemical Shifts

These increments are added to the shift value of the appropriate carbon atom as calculated from Table 7.50.



| Substituent group Y*      | $\alpha$ carbon |          | $\beta$ carbon |          | $\gamma$ carbon |
|---------------------------|-----------------|----------|----------------|----------|-----------------|
|                           | Straight        | Branched | Straight       | Branched |                 |
| —CO—OH                    | 20.9            | 16       | 2.5            | 2        | − 2.2           |
| —COO <sup>−</sup> (anion) | 24.4            | 20       | 4.1            | 3        | − 1.6           |
| —CO—OR                    | 20.5            | 17       | 2.5            | 2        | − 2             |
| —CO—Cl                    | 33              | 28       |                | 2        |                 |
| —CO—NH <sub>2</sub>       | 22              | 2.5      |                |          | − 0.5           |
| —CHO                      | 31              |          | 0              |          | − 2             |
| —CO—R                     | 30              | 24       | 1              | 1        | − 2             |
| —OH                       | 48.3            | 40.8     | 10.2           | 7.7      | − 5.8           |
| —OR                       | 58              | 51       | 8              | 5        | − 4             |
| —O—CO—NH <sub>2</sub>     | 51              |          | 8              |          |                 |
| —O—CO—R                   | 51              | 45       | 6              | 5        | − 3             |
| —C—CO—Ar                  | 53              |          |                |          |                 |
| —F                        | 68              | 63       | 9              | 6        | − 4             |
| —Cl                       | 31.2            | 32       | 10.5           | 10       | − 4.6           |
| —Br                       | 20.0            | 25       | 10.6           | 10       | − 3.1           |

\* R, alkyl group; Ar, aryl group.

**TABLE 7.51** Effect of Substituent Groups on Alkyl Chemical Shifts (*Continued*)

| Substituent group Y*           | $\alpha$ carbon |          | $\beta$ carbon |          | $\gamma$ carbon |
|--------------------------------|-----------------|----------|----------------|----------|-----------------|
|                                | Straight        | Branched | Straight       | Branched |                 |
| —I                             | —8              | 4        | 11.3           | 12       | —1.0            |
| —NH <sub>2</sub>               | 29.3            | 24       | 11.3           | 10       | —4.6            |
| —NH <sub>3</sub> <sup>+</sup>  | 26              | 24       | 8              | 6        | —5              |
| —NHR                           | 36.9            | 31       | 8.3            | 6        | —3.5            |
| —NR <sub>2</sub>               | 42              |          | 6              |          | —3              |
| —NR <sub>3</sub> <sup>+</sup>  | 31              |          | 5              |          | —7              |
| —NO <sub>2</sub>               | 63              | 57       | 4              | 4        |                 |
| —CN                            | 4               | 1        | 3              | 3        | —3              |
| —SH                            | 11              | 11       | 12             | 11       | —6              |
| —SR                            | 20              |          | 7              |          | —3              |
| —CH=CH <sub>2</sub>            | 20              |          | 6              |          | —0.5            |
| —C <sub>6</sub> H <sub>5</sub> | 23              | 17       | 9              | 7        | —2              |
| —C≡CH                          | 4.5             |          | 5.5            |          | —3.5            |

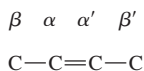
\* R, alkyl group; Ar, aryl group.

**TABLE 7.52** Estimation of Chemical Shifts of Carbon Attached to a Double Bond

The olefinic carbon chemical shift is calculated from the equation

$$\delta_C = 123.3 + 10.6n_\alpha + 7.2n_\beta - 7.9n_\alpha - 1.8n_\beta \quad (\text{plus any steric correction terms})$$

where  $n$  is the number of carbon atoms at the particular position, namely,



Substituents on both sides of the double bond are considered separately. Additional vinyl carbons are treated as if they were alkyl carbons. The method is applicable to alicyclic alkenes; in small rings carbons are counted twice, i.e., from both sides of the double bond where applicable. The constant in the equation is the chemical shift for ethylene. The effect of other substituent groups is tabulated below.

| Substituent group              | $\beta$ | $\alpha$ | $\alpha'$ | $\beta'$ |
|--------------------------------|---------|----------|-----------|----------|
| —OR                            | 2       | 29       | —39       | —1       |
| —OH                            | 6       |          |           | —1       |
| —O—CO—CH <sub>3</sub>          | —3      | 18       | —27       | 4        |
| —CO—CH <sub>3</sub>            |         | 15       | 6         |          |
| —CHO                           |         | 13.6     | 13.2      |          |
| —CO—OH                         |         | 5.2      | 9.1       |          |
| —CO—OR                         |         | 6        | 7         |          |
| —CN                            |         | —15.4    | 14.3      |          |
| —F                             |         | 24.9     | —34.3     |          |
| —Cl                            | —1      | 3.3      | —5.4      | 2        |
| —Br                            | 0       | —7.2     | —0.7      | 2        |
| —I                             |         | —37.4    | 7.7       |          |
| —C <sub>6</sub> H <sub>5</sub> |         | 12       | —11       |          |

**TABLE 7.52** Estimation of Chemical Shifts of Carbon Attached to a Double Bond (*Continued*)

| Substituent pair   |              | Steric correction term |
|--------------------|--------------|------------------------|
| $\alpha, \alpha'$  | <i>trans</i> | 0                      |
| $\alpha, \alpha'$  | <i>cis</i>   | −1.1                   |
| $\alpha, \alpha$   | <i>gem</i>   | −4.8                   |
| $\alpha', \alpha'$ |              | +2.5                   |
| $\beta, \beta$     |              | +2.3                   |

**TABLE 7.53** Carbon-13 Chemical Shifts in Substituted Benzenes

$$\delta_C = 128.5 + \Delta$$

| Substituent group                               | $\Delta_{C-1}$ | $\Delta_{ortho}$ | $\Delta_{meta}$ | $\Delta_{para}$ |
|-------------------------------------------------|----------------|------------------|-----------------|-----------------|
| —CH <sub>3</sub>                                | 9.3            | 0.8              | −0.1            | −2.9            |
| —CH <sub>2</sub> CH <sub>3</sub>                | 15.6           | −0.4             | 0               | −2.6            |
| —CH(CH <sub>3</sub> ) <sub>2</sub>              | 20.2           | −2.5             | 0.1             | −2.4            |
| —C(CH <sub>3</sub> ) <sub>3</sub>               | 22.4           | −3.1             | −0.1            | −2.9            |
| —CH <sub>2</sub> O—CO—CH <sub>3</sub>           | 7.7            | 0                | 0               | 0               |
| —C <sub>6</sub> H <sub>5</sub>                  | 13.1           | −1.1             | 0.4             | −1.2            |
| —CH=CH <sub>2</sub>                             | 9.5            | −2.0             | 0.2             | −0.5            |
| —C≡CH                                           | −6.1           | 3.8              | 0.4             | −0.2            |
| —CH <sub>2</sub> OH                             | 12.3           | −1.4             | −1.4            | −1.4            |
| —CO—OH                                          | 2.1            | 1.5              | 0               | 5.1             |
| —COO <sup>−</sup> (anion)                       | 8              | 1                | 0               | 3               |
| —CO—OCH <sub>3</sub>                            | 2.1            | 1.1              | 0.1             | 4.5             |
| —CO—CH <sub>3</sub>                             | 9.1            | 0.1              | 0               | 4.2             |
| —CHO                                            | 8.6            | 1.3              | 0.6             | 5.5             |
| —CO—Cl                                          | 4.6            | 2.4              | 1               | 6.2             |
| —CO—CF <sub>3</sub>                             | −5.6           | 1.8              | 0.7             | 6.7             |
| —CO—C <sub>6</sub> H <sub>5</sub>               | 9.4            | 1.7              | −0.2            | 3.6             |
| —CN                                             | −15.4          | 3.6              | 0.6             | 3.9             |
| —OH                                             | 26.9           | −12.7            | 1.4             | −7.3            |
| —OCH <sub>3</sub>                               | 31.4           | −14.0            | 1.0             | −7.7            |
| —OC <sub>6</sub> H <sub>5</sub>                 | 29.2           | −9.4             | 1.6             | −5.1            |
| —O—CO—CH <sub>3</sub>                           | 23.0           | −6.4             | 1.3             | −2.3            |
| —NH <sub>2</sub>                                | 18.0           | −13.3            | 0.9             | −9.8            |
| —N(CH <sub>3</sub> ) <sub>2</sub>               | 22.4           | −15.7            | 0.8             | −11.5           |
| —N(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> | 19             | −4               | 1               | −6              |
| —NHC <sub>6</sub> H <sub>5</sub>                | 14.6           | −10.7            | 0.7             | −7.7            |
| —NH—CO—CH <sub>3</sub>                          | 11.1           | −9.9             | 0.2             | −5.6            |
| —NO <sub>2</sub>                                | 20.0           | −4.8             | 0.9             | 5.8             |
| —F                                              | 34.8           | −12.9            | 1.4             | −4.5            |
| —Cl                                             | 6.2            | 0.4              | 1.3             | −1.9            |
| —Br                                             | −5.5           | 3.4              | 1.7             | −1.6            |
| —I                                              | −32.2          | 9.9              | 2.6             | −1.4            |
| —CF <sub>3</sub>                                | −9.0           | −2.2             | 0.3             | 3.2             |
| —NCO                                            | 5.7            | −3.6             | 1.2             | −2.8            |
| —SH                                             | 2.3            | 1.1              | 1.1             | −3.1            |
| —SCH <sub>3</sub>                               | 10.2           | −1.8             | 0.4             | −3.6            |
| —SO <sub>2</sub> —NH <sub>2</sub>               | 15.3           | −2.9             | 0.4             | 3.3             |
| —Si(CH <sub>3</sub> ) <sub>3</sub>              | 13.4           | 4.4              | −1.1            | −1.1            |

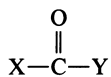
**TABLE 7.54** Carbon-13 Chemical Shifts in Substituted Pyridines\*

$$\delta_C(k) = C_k + \Delta_i$$

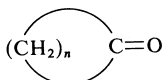
| Substituent group                | $C_2 = C_6 = 149.6$<br>$\Delta_{C-2} \text{ or } \Delta_{C-6}$ |                                                                | $\Delta_{23}$               | $\Delta_{24}$ | $\Delta_{25}$                   | $\Delta_{26}$ |
|----------------------------------|----------------------------------------------------------------|----------------------------------------------------------------|-----------------------------|---------------|---------------------------------|---------------|
| —CH <sub>3</sub>                 | 9.1                                                            |                                                                | −1.0                        | −0.1          | −3.4                            | −0.1          |
| —CH <sub>2</sub> CH <sub>3</sub> | 14.0                                                           |                                                                | −2.1                        | 0.1           | −3.1                            | 0.2           |
| —CO—CH <sub>3</sub>              | 4.3                                                            |                                                                | −2.8                        | 0.7           | 3.0                             | −0.2          |
| —CHO                             | 3.5                                                            |                                                                | −2.6                        | 1.3           | 4.1                             | 0.7           |
| —OH                              | 14.9                                                           |                                                                | −17.2                       | 0.4           | −3.1                            | −6.8          |
| —OCH <sub>3</sub>                | 15.3                                                           |                                                                | −13.1                       | 2.1           | −7.5                            | −2.2          |
| —NH <sub>2</sub>                 | 11.3                                                           |                                                                | −14.7                       | 2.3           | 10.6                            | −0.9          |
| —NO <sub>2</sub>                 | 8.0                                                            |                                                                | −5.1                        | 5.5           | 6.6                             | 0.4           |
| —CN                              | −15.8                                                          |                                                                | −5.0                        | −1.7          | 3.6                             | 1.9           |
| —F                               | 14.4                                                           |                                                                | −14.7                       | 5.1           | −2.7                            | −1.7          |
| —Cl                              | 2.3                                                            |                                                                | 0.7                         | 3.3           | −1.2                            | 0.6           |
| —Br                              | −6.7                                                           |                                                                | 4.8                         | 3.3           | −0.5                            | 1.4           |
| Substituent group                | $\Delta_{32}$                                                  | $C_3 = C_5 = 124.2$<br>$\Delta_{C-3} \text{ or } \Delta_{C-5}$ | $\Delta_{34}$               | $\Delta_{35}$ |                                 |               |
| —CH <sub>3</sub>                 | 1.3                                                            | 9.0                                                            | 0.2                         | −0.8          | −2.3                            |               |
| —CH <sub>2</sub> CH <sub>3</sub> | 0.3                                                            | 15.0                                                           | −1.5                        | −0.3          | −1.8                            |               |
| —CO—CH <sub>3</sub>              | 0.5                                                            | −0.3                                                           | −3.7                        | −2.7          | 4.2                             |               |
| —CHO                             | 2.4                                                            | 7.9                                                            | 0                           | 0.6           | 5.4                             |               |
| —OH                              | −10.7                                                          | 31.4                                                           | −12.2                       | 1.3           | −8.6                            |               |
| —NH <sub>2</sub>                 | −11.9                                                          | 21.5                                                           | −14.2                       | 0.9           | −10.8                           |               |
| —CN                              | 3.6                                                            | −13.7                                                          | 4.4                         | 0.6           | 4.2                             |               |
| —Cl                              | −0.3                                                           | 8.2                                                            | −0.2                        | 0.7           | −1.4                            |               |
| —Br                              | 2.1                                                            | −2.6                                                           | 2.9                         | 1.2           | −0.9                            |               |
| —I                               | 7.1                                                            | −28.4                                                          | 9.1                         | 2.4           | 0.3                             |               |
| Substituent group                | $\Delta_{42} = \Delta_{46}$                                    |                                                                | $\Delta_{43} = \Delta_{45}$ |               | $C_4 = 136.2$<br>$\Delta_{C-4}$ |               |
| —CH <sub>3</sub>                 | 0.5                                                            |                                                                | 0.8                         |               | 10.8                            |               |
| —CH <sub>2</sub> CH <sub>3</sub> | 0                                                              |                                                                | −0.3                        |               | 15.9                            |               |
| —CH=CH <sub>2</sub>              | 0.3                                                            |                                                                | −2.9                        |               | 8.6                             |               |
| —CO—CH <sub>3</sub>              | 1.6                                                            |                                                                | −2.6                        |               | 6.8                             |               |
| —CHO                             | 1.7                                                            |                                                                | −0.6                        |               | 5.5                             |               |
| —NH <sub>2</sub>                 | 0.9                                                            |                                                                | −13.8                       |               | 19.6                            |               |
| —CN                              | 2.1                                                            |                                                                | 2.2                         |               | −15.7                           |               |
| —Br                              | 3.0                                                            |                                                                | 3.4                         |               | −3.0                            |               |

\* May be used for disubstituted, polyheterocyclic, and polynuclear systems if deviations due to steric and mesomeric effects are allowed for.

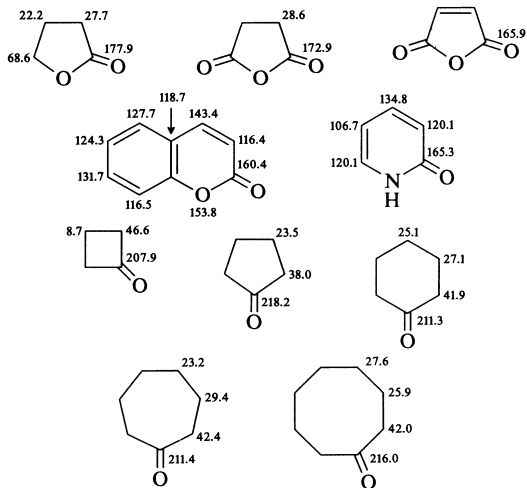


**TABLE 7.55** Carbon-13 Chemical Shifts of Carbonyl Group

| X                                        | Y                                     | $\delta_{\text{C}}$ | X                 | Y                                                                  | $\delta_{\text{C}}$ |
|------------------------------------------|---------------------------------------|---------------------|-------------------|--------------------------------------------------------------------|---------------------|
| H—                                       | —CH <sub>3</sub>                      | 199.7               | CH <sub>3</sub> — | —CH=CH <sub>2</sub>                                                | 196.9               |
| H—                                       | —CCl <sub>3</sub>                     | 175.3               | CH <sub>3</sub> — | —C <sub>6</sub> H <sub>5</sub>                                     | 197.6               |
| H—                                       | —NH <sub>2</sub>                      | 165.5               | CH <sub>3</sub> — | —CH <sub>2</sub> —CO—CH <sub>3</sub>                               | 201.9               |
|                                          |                                       |                     |                   | (keto)                                                             |                     |
| H—                                       | —N(CH <sub>3</sub> ) <sub>2</sub>     | 162.4               |                   |                                                                    | 191.4               |
|                                          |                                       |                     |                   | (enol)                                                             |                     |
| H—                                       | 2-Furyl                               | 153.3               | CH <sub>3</sub> — | —CH <sub>2</sub> CHO                                               | 167.7               |
| H—                                       | 2-Pyrrolyl                            | 134.0               | CH <sub>3</sub> — | —C <sub>6</sub> H <sub>5</sub> —CH <sub>3</sub>                    | 196 ( <i>m, p</i> ) |
| H—                                       | 2-Thienyl                             | 143.3               |                   |                                                                    | 199 ( <i>o</i> )    |
| (CH <sub>3</sub> ) <sub>2</sub> CH—      | —OH                                   | 184.8               | CH <sub>3</sub> — | —2,6-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> | 206                 |
| C <sub>6</sub> H <sub>5</sub> —          | —OH                                   | 172.6               | CH <sub>3</sub> — | —OH                                                                | 178                 |
| CF <sub>3</sub> —                        | —OH                                   | 163.0               | CH <sub>3</sub> — | —O <sup>−</sup> (anion)                                            | 181.5               |
| CCl <sub>3</sub> —                       | —OH                                   | 168.0               | CH <sub>3</sub> — | —OCH <sub>3</sub>                                                  | 170.7               |
| CH <sub>3</sub> CH(NH <sub>2</sub> )—    | —OH                                   | 176.5               | CH <sub>3</sub> — | —O—CH=CH <sub>2</sub>                                              | 167.7               |
| CF <sub>3</sub> —                        | —OCH <sub>2</sub> CH <sub>3</sub>     | 158.1               | CH <sub>3</sub> — | —O—CH(CH <sub>3</sub> ) <sub>2</sub>                               | 170.3               |
| H <sub>2</sub> N—                        | —OCH <sub>2</sub> CH <sub>3</sub>     | 157.8               | CH <sub>3</sub> — | —O—CO—CH <sub>3</sub>                                              | 167.3               |
| 2-Furyl                                  | —OCH <sub>3</sub>                     | 159.1               | CH <sub>3</sub> — | —NH <sub>2</sub>                                                   | 172.7               |
| (CH <sub>3</sub> ) <sub>2</sub> N—       | —C <sub>6</sub> H <sub>5</sub>        | 170.8               | CH <sub>3</sub> — | —NHCH <sub>3</sub>                                                 | 172                 |
| CH <sub>2</sub> =CHCH <sub>2</sub> O—CO— | —OCH <sub>2</sub> CH=CH <sub>2</sub>  | 157.6               | CH <sub>3</sub> — | —N(CH <sub>3</sub> ) <sub>2</sub>                                  | 169.5               |
| CH <sub>3</sub> CH <sub>2</sub> —        | —CH <sub>2</sub> CH <sub>3</sub>      | 211.4               | CH <sub>3</sub> — | —Cl                                                                | 169.6               |
| CH <sub>3</sub> —CH <sub>2</sub> —       | —O—CO—CH <sub>2</sub> CH <sub>3</sub> | 170.3               | CH <sub>3</sub> — | —Br                                                                | 165.6               |
| CH <sub>3</sub> —                        | —CH <sub>3</sub>                      | 205.8               | CH <sub>3</sub> — | —I                                                                 | 158.9               |
| CH <sub>3</sub> —                        | —CH <sub>2</sub> CH <sub>3</sub>      | 207                 |                   |                                                                    |                     |



| <i>n</i> | $\delta_{\text{C}}$ |
|----------|---------------------|
| 3        | 207.9               |
| 4        | 218.2               |
| 5        | 211.3               |
| 6        | 211.4               |
| 7        | 216.0               |



**TABLE 7.56** One-Bond Carbon-Hydrogen Spin Coupling Constants

[illegible]

TABLE 7.56 One-Bond Carbon-Hydrogen Spin Coupling Constants (Continued)

| Structure                                                                                  | $J_{\text{CH}}$ , Hz | Structure                                                                         | $J_{\text{CH}}$ , Hz |
|--------------------------------------------------------------------------------------------|----------------------|-----------------------------------------------------------------------------------|----------------------|
| <br>2<br>4 | 208<br>199           |  | 216                  |
|            | 205                  |                                                                                   |                      |

TABLE 7.57 Two-Bond Carbon-Hydrogen Spin Coupling Constants

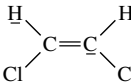
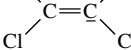
| Structure                             | $^2J_{\text{CH}}$ , Hz | Structure                                                                                      | $^2J_{\text{CH}}$ , Hz |
|---------------------------------------|------------------------|------------------------------------------------------------------------------------------------|------------------------|
| $\text{CH}_3\text{—CH}_2\text{—H}$    | −4.5                   | $(\text{CH}_2)_n\text{C=CH}_2$ $n = 4$                                                         | 4.2                    |
| $\text{CCl}_3\text{—CH}_2\text{—H}$   | 5.9                    | $(\text{CH}_2)_n\text{C=CH}_2$ $n = 5$                                                         | 5.2                    |
| $\text{ClCH}_2\text{—CH}_2\text{Cl}$  | −3.4                   | $(\text{CH}_2)_n\text{C=CH}_2$ $n = 6$                                                         | 5.5                    |
| $\text{Cl}_2\text{CH—CHCl}_2$         | 1.2                    |  <i>cis</i>   | 16.0                   |
| $\text{CH}_3\text{—CHO}$              | 26.7                   |  <i>trans</i> | 0.8                    |
| $\text{CH}_2\text{=CH}_2$             | −2.4                   | $\text{HC}\equiv\text{CH}$                                                                     | 49.3                   |
| $(\text{CH}_3)_2\text{C=O}$           | 5.5                    | $\text{C}_6\text{H}_5\text{O—C}\equiv\text{CH}$                                                | 61.0                   |
| $\text{CH}_2\text{=CH—CH=O}$          | 26.9                   | $\text{HC}\equiv\text{C—CHO}$                                                                  | 33.2                   |
| $(\text{C}_2\text{H}_5)\text{CH—CHO}$ | 26.9                   | $\text{ClCH}_2\text{—CHO}$                                                                     | 32.5                   |
| $\text{H}_2\text{NCH=CH—CHO}$         | 6.0                    | $\text{Cl}_2\text{CH—CHO}$                                                                     | 35.3                   |
| $\text{H}_2\text{NCH—CH—CHO}$         | 20.0                   | $\text{Cl}_3\text{C—CHO}$                                                                      | 46.3                   |
| $\text{C}_6\text{H}_6$                | 1.0                    | $\text{C}_6\text{H}_5\text{—C}\equiv\text{C}\equiv\text{CH}_3$                                 | 10.8                   |

TABLE 7.58 Carbon-Carbon Spin Coupling Constants

| Structure*                                     | $J_{\text{CC}}$ , Hz | Structure                                           | $J_{\text{CC}}$ , Hz |
|------------------------------------------------|----------------------|-----------------------------------------------------|----------------------|
| $\text{H}_3\text{C—CH}_3$                      | 35                   | $\text{C—CO—OR}$                                    | 59                   |
| $\text{H}_3\text{C—CHR}_2$                     | 37                   | $\text{C—CN}$                                       | 52–57                |
| $\text{H}_3\text{C—CH}_2\text{Ar}$             | 34                   | $\text{C—C}\equiv\text{C}$ $^2J_{\text{CC}} = 11.8$ | 67                   |
| $\text{H}_3\text{C—CH}_2\text{CN}$             | 33                   | $\text{H}_2\text{C=CH}_2$                           | 68                   |
| $\text{H}_3\text{C—CH}_2\text{—CH}_2\text{OH}$ |                      | $\text{>C=C—CO—OH}$                                 | 70–71                |
| C-1, C-2                                       | 38                   | $\text{>C=C—CN}$                                    | 71                   |
| C-2, C-3                                       | 34                   | $\text{>C=C—Ar}$                                    | 67–70                |
| $\text{H}_3\text{C—CH}_2\text{NH}_2$           | 37                   | $\text{C}_6\text{H}_6$                              | 57                   |
| $\text{C—C=O}$                                 | 38–40                | $\text{C}_3\text{H}_5\text{NO}_2$                   |                      |
| $\text{C—C—C=O}$                               | 36                   | 1-2                                                 | 55                   |
| $\text{C—C—Ar}$                                | 43                   | 2-3, 3-4                                            | 56                   |
| $\text{C—CO—O}^-$ (anion)                      | 52                   | $^3J_{2-5}$                                         | 7.6                  |
| $\text{C—CO—N}$                                | 52                   |                                                     |                      |
| $\text{C—CO—OH}$                               | 57                   |                                                     |                      |

\* R, alkyl group; Ar, aryl group.

**TABLE 7.58** Carbon-Carbon Spin Coupling Constants (*Continued*)

| Structure*     | $J_{CC}$ , Hz | Structure                              | $J_{CC}$ , Hz   |
|----------------|---------------|----------------------------------------|-----------------|
| $C_6H_5I$      |               | Pyridine                               |                 |
| 1-2            | 60            | 2-3                                    | 54              |
| 2-3            | 53            | 3-4                                    | 56              |
| 3-4            | 58            | $^3J_{2,5}$                            | 14              |
| $^3J_{2,5}$    | 8.6           | Furan                                  | 69              |
| $C_6H_5-OCH_3$ |               | Pyrrole                                | 69              |
| 2-3            | 58            | Thiophene                              | 64              |
| 3-4            | 56            | $H_2C=C=C(CH_3)_2$                     | 100             |
| $C_6H_5NH_2$   |               | $-C\equiv C-$                          | 170–176         |
| 1-2            | 61            |                                        |                 |
| 2-3            | 58            | Structure                              | $^2J_{CC}$ , Hz |
| 3-4            | 57            |                                        |                 |
| $^3J_{2,5}$    | 7.9           | $CH_3-CO=CH_3$                         | 16              |
| $C_6H_5CH_3$   | 44            | $\overline{CH}_3-C\equiv\overline{CH}$ | 11.8            |
|                |               | $\overline{CH}_3CH_2-\overline{CN}$    | 33              |

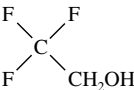
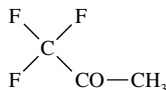
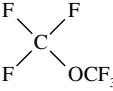
\* R, alkyl group; Ar, aryl group.

**TABLE 7.59** Carbon-Fluorine Spin Coupling Constants

| Structure*                | $J_{CF}$ , Hz | Structure*           | $J_{CF}$ , Hz |
|---------------------------|---------------|----------------------|---------------|
|                           | –158          | $p-F-C_6H_4-CF_3$    | –252          |
|                           | –235          | $p-F-C_6H_4-CO-CH_3$ | –253          |
|                           | –274          | $p-F-C_6H_4-NO_2$    | –257          |
|                           | –259          | $F-C_6H_5$           | –244          |
|                           | –271          | $^2J_{CF} = 21.0$    |               |
|                           | –165          | $^3J_{CF} = 7.7$     |               |
| $F-CH_2CH_2-$ or $F-CR_3$ | –167          | $^4J_{CF} = 3.4$     |               |
| $p-F-C_6H_4-OR$           | –237          |                      | –287          |
| $p-F-C_6H_4-R$            | –241          |                      | –308          |
|                           |               |                      | –353          |
|                           |               |                      | –369          |
|                           |               |                      | –241          |

\* Ar, aryl group; R, alkyl group.

TABLE 7.59 Carbon-Fluorine Spin Coupling Constants (*Continued*)

| Structure*                                                                       | $J_{\text{CF}}$ , Hz | Structure*                                                                        | $J_{\text{CF}}$ , Hz |
|----------------------------------------------------------------------------------|----------------------|-----------------------------------------------------------------------------------|----------------------|
|  | -278                 |  | -289                 |
|  | -265                 |                                                                                   |                      |

\* Ar, aryl group; R, alkyl group.

TABLE 7.60 Carbon-13 Chemical Shifts of Deuterated Solvents  
*Relative to tetramethylsilane.*

| Solvent                   | Group                           | $\delta$ , ppm |
|---------------------------|---------------------------------|----------------|
| Acetic- $d_3$ acid- $d_1$ | Methyl                          | 20.0           |
|                           | Carbonyl                        | 205.8          |
| Acetone- $d_6$            | Methyl                          | 28.1           |
|                           | Carbonyl                        | 178.4          |
| Acetonitrile- $d_3$       | Methyl                          | 1.3            |
|                           | Carbonyl                        | 117.7          |
| Benzene- $d_6$            |                                 | 128.5          |
| Carbon disulfide          |                                 | 193            |
| Carbon tetrachloride      |                                 | 97             |
| Chloroform- $d_1$         |                                 | 77             |
| Cyclohexane- $d_{12}$     |                                 | 25.2           |
| Dimethyl sulfoxide- $d_6$ |                                 | 39.5           |
| 1,4-Dioxane- $d_6$        |                                 | 67             |
| Formic- $d_1$ acid- $d_1$ | Carbonyl                        | 165.5          |
| Methanol- $d_4$           |                                 | 47–49          |
| Methylene chloride- $d_2$ |                                 | 53.8           |
| Nitromethane- $d_3$       |                                 | 57.3           |
| Pyridine- $d_5$           | C <sub>3</sub> , C <sub>5</sub> | 123.5          |
|                           | C <sub>4</sub>                  | 135.5          |
|                           | C <sub>2</sub> , C <sub>6</sub> | 149.9          |

TABLE 7.61 Carbon-13 Spin Coupling Constants with Various Nuclei

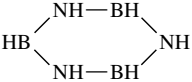
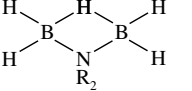
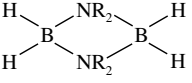
| Nuclei       | Structure                    | $^1J$ , Hz | $^2J$ , Hz | $^3J$ , Hz | $^4J$ , Hz |
|--------------|------------------------------|------------|------------|------------|------------|
| $^2\text{H}$ | $\text{CDCl}_3$              | 32         |            |            |            |
|              | $\text{CD}_3\text{—CO—CD}_3$ | 20         |            |            |            |
|              | $(\text{CD}_3)_2\text{SO}$   | 22         |            |            |            |
|              | $\text{C}_6\text{D}_6$       | 26         |            |            |            |

**TABLE 7.61** Carbon-13 Spin Coupling Constants with Various Nuclei (*Continued*)

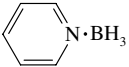
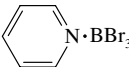
| Nuclei            | Structure                                           | $^1J$ , Hz | $^2J$ , Hz | $^3J$ , Hz | $^4J$ , Hz |
|-------------------|-----------------------------------------------------|------------|------------|------------|------------|
| $^7\text{Li}$     | $\text{CH}_3\text{Li}$                              | 15         |            |            |            |
| $^{11}\text{B}$   | $(\text{C}_6\text{H}_5)_4\text{B}^-$                | 49         |            | 3          |            |
| $^{14}\text{N}$   | $(\text{CH}_3)_4\text{N}^+$                         | 10         |            |            |            |
|                   | $\text{CH}_3\text{NC}$                              | 8          |            |            |            |
| $^{29}\text{Si}$  | $(\text{CH}_3)_4\text{Si}$                          | 52         |            |            |            |
| $^{31}\text{P}$   | $(\text{CH}_3)_3\text{P}$                           | 14         |            |            |            |
|                   | $(\text{C}_4\text{H}_9)_3\text{P}$                  | 11         | 12         | 5          |            |
|                   | $(\text{C}_6\text{H}_5)_3\text{P}$                  | 12         | 20         | 7          | 0          |
|                   | $(\text{CH}_3)_4\text{P}^+$                         | 56         |            |            |            |
|                   | $(\text{C}_4\text{H}_9)_4\text{P}^+$                | 48         | 4          | 15         |            |
|                   | $(\text{C}_6\text{H}_5)_4\text{P}^+$                | 88         | 11         | 13         | 3          |
|                   | $\text{R}(\text{RO})_2\text{P}=\text{O}$            | 142        | 5–7        |            |            |
|                   | $(\text{C}_4\text{H}_9\text{O})_3\text{P}=\text{O}$ |            | 6          | 7          |            |
| $^{77}\text{Se}$  | $(\text{CH}_3)_2\text{Se}$                          | 62         |            |            |            |
|                   | $(\text{CH}_3)_3\text{Se}^+$                        | 50         |            |            |            |
| $^{113}\text{Cd}$ | $(\text{CH}_3)_2\text{Cd}$                          | 513, 537   |            |            |            |
| $^{119}\text{Sn}$ | $(\text{CH}_3)_4\text{Sn}$                          | 340        |            |            |            |
|                   | $(\text{CH}_3)_3\text{SnC}_6\text{H}_5$             | 474        | 37         | 47         | 11         |
| $^{125}\text{Te}$ | $(\text{CH}_3)_2\text{Te}$                          | 162        |            |            |            |
| $^{199}\text{Hg}$ | $(\text{CH}_3)_2\text{Hg}$                          | 687        |            |            |            |
|                   | $(\text{C}_6\text{H}_5)_2\text{Hg}$                 | 1186       | 88         | 102        | 18         |
| $^{207}\text{Pb}$ | $(\text{CH}_3)_2\text{Pb}$                          | 250        |            |            |            |
|                   | $(\text{C}_6\text{H}_5)_4\text{Pb}$                 | 481        | 68         | 81         | 20         |

**TABLE 7.62** Boron-11 Chemical Shifts

Values given in ppm on the  $\delta$  scale, relative to  $\text{B}(\text{OCH}_3)_3$ .

| Structure                                   | $\delta$ , ppm | Structure                                                                           | $\delta$ , ppm |
|---------------------------------------------|----------------|-------------------------------------------------------------------------------------|----------------|
| $\text{R}_3\text{B}$                        | –67 to –68     |  | –12            |
| $\text{Ar}_3\text{B}$                       | –43            |                                                                                     |                |
| $\text{BF}_3$                               | 24             |  | 37             |
| $\text{BCl}_3$                              | –12            |                                                                                     |                |
| $\text{BBr}_3$                              | –6             |                                                                                     |                |
| $\text{BI}_3$                               | 41             |                                                                                     |                |
| $\text{B}(\text{OH})_3$                     | 36             |  | 15             |
| $\text{B}(\text{OR})_3$                     | 0–1            |                                                                                     |                |
| $\text{B}(\text{NR}_2)_3$                   | –13            |                                                                                     |                |
| $\text{C}_6\text{H}_5\text{BCl}_2$          | –36            |                                                                                     |                |
| $\text{C}_6\text{H}_5\text{B}(\text{OH})_2$ | –14            |                                                                                     |                |
| $\text{C}_6\text{H}_5\text{B}(\text{OR})_2$ | –10            |                                                                                     |                |
| $\text{M}(\text{BH}_4)$                     | 55–61          | $(\text{CH}_3)_2\text{N}-\text{B}(\text{CH}_3)_2$                                   | 62             |
| $\text{B}(\text{BF}_4)$                     | 19–20          |                                                                                     |                |

**TABLE 7.62** Boron-11 Chemical Shifts (*Continued*)

| Structure                                                                        | $\delta$ , ppm | Structure      | $\delta$ , ppm |      |
|----------------------------------------------------------------------------------|----------------|----------------|----------------|------|
| <b>Addition complexes</b>                                                        |                | <b>Boranes</b> |                |      |
| $R_2O \cdot BH_3$                                                                | 18–19          | $B_2H_6$       | 1              |      |
| $R_3N \cdot BH_3$                                                                | 25             | $B_3H_{10}$    | 25             |      |
| $R_2NH \cdot BH_3$                                                               | 33             | ( $BH_2$ )     | 60             |      |
|  | 31             | (BH)           |                |      |
| $R_2O(\text{or ROH}) \cdot BF_3$                                                 | 17–19          |                | Base           | Apex |
| $R_2O(\text{or ROH}) \cdot BCl_3$                                                | –7 to –8       | $B_5H_9$       | 31             | 70   |
| $R_2O(\text{or ROH}) \cdot BBr_3$                                                | 23–24          | $B_3H_{11}$    | –16            | 50   |
| $R_2O(\text{or ROH}) \cdot BI_3$                                                 | 74–82          | $B_{10}H_{14}$ | 7              | 54   |
|  | 24             |                |                |      |

**TABLE 7.63** Nitrogen-15 (or Nitrogen-14) Chemical Shifts

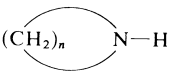
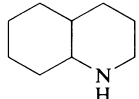
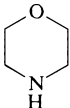
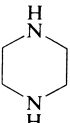
Values given in ppm on the  $\delta$  scale, relative to  $NH_3$  liquid.

| Substituent group                | $\delta$ , ppm | Substituent group                   | $\delta$ , ppm |
|----------------------------------|----------------|-------------------------------------|----------------|
| <b>Aliphatic amines</b>          |                | <b>Amides (<i>continued</i>)</b>    |                |
| Primary                          | 1–59           | $HCO-NH-Aryl$                       | 138–141        |
| Secondary                        | 7–81           | $RCO-NHR$ or $RCO-NR_2$             | 103–130        |
| Tertiary                         | 14–44          | $RCO-NH-Aryl$                       | 131–136        |
| Cyclo, primary                   | 29–44          | $Aryl-CO-H-Aryl$                    | ca 126         |
| Aryl amines                      | 40–100         | <b>Guanidines</b>                   |                |
| Aryl hydrazines                  | 40–100         | Amino                               | 30–60          |
| Piperidines, decahydroquinolines | 30–82          | Imino                               | 166–207        |
| <b>Amine cations</b>             |                | Thioureas                           | 85–111         |
| Primary                          | 19–59          | Thioamides                          | 135–154        |
| Secondary                        | 40–74          | <b>Cyanamides</b>                   |                |
| Tertiary                         | 30–67          | $R_2N-$                             | –12 to –38     |
| Quaternary                       | 43–70          | $-CN$                               | 175–200        |
| <b>Enamines, tertiary type</b>   |                | <b>Carbodiimides</b>                | 95–120         |
| Alkyl                            | 29–82          | <b>Isocyanates</b>                  |                |
| Cycloalkyl                       | 55–104         | Alkyl, primary                      | 14–32          |
| <b>Aminophosphines</b>           | 59–100         | Alkyl, secondary and tertiary       | 54–57          |
| <b>Amine N-oxides</b>            | 95–122         | Aryl                                | ca 46          |
| <b>Ureas</b>                     |                | <b>Isothiocyanates</b>              | 90–107         |
| Aliphatic                        | 63–84          | <b>Azides</b>                       | 52–80          |
| Aryl                             | 105–108        |                                     | 108–122        |
| <b>Sulfonamides</b>              | 79–164         |                                     | 240–260        |
| <b>Amides</b>                    |                | <b>Lactams</b>                      | 113–122        |
| $HCO-NHR$                        |                | <b>Hydrazones</b>                   |                |
| R = primary                      | 100–115        | Amino                               | 141–167        |
| R = secondary                    | 104–148        | Imino                               | 319–327        |
| R = tertiary                     | 96–133         | Cyanates                            | 155–182        |
|                                  |                | <b>Nitrile N-oxides, fulminates</b> | 195–225        |

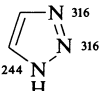
**TABLE 7.63** Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*Continued*)

| Substituent group      | $\delta$ , ppm | Substituent group            | $\delta$ , ppm |
|------------------------|----------------|------------------------------|----------------|
| Isonitriles            |                | Oximes                       | 340–380        |
| Alkyl, primary         | 162–178        | Nitramines                   |                |
| Alkyl, secondary       | 191–199        | Amine                        | 252–280        |
| Aryl                   | ca 180         | —NO <sub>2</sub>             | 328–355        |
| Nitriles               |                | Nitrates                     | 310–353        |
| Alkyl                  | 235–241        | <i>gem</i> -Polynitroalkanes | 310–353        |
| Aryl                   | 258–268        | Nitro                        |                |
| Thiocyanates           | 265–280        | Aryl                         | 350–382        |
| Diazonium              |                | Alkyl                        | 372–410        |
| Internal               | 222–230        | Hetero, unsaturated          | 354–367        |
| Terminal               | 315–322        | Azoxy                        | 330–356        |
| Diazo                  |                | Azo                          | 504–570        |
| Internal               | 226–303        | Nitrosamines                 | 222–250        |
| Terminal               | 315–440        |                              | 525–550        |
| Nitrilium ions         | 123–150        | Nitrites                     | 555–582        |
| Azinium ions           | 185–220        | Thionitrites                 | 720–790        |
| Azine <i>N</i> -oxides | 230–300        | Nitroso                      |                |
| Nitrones               | 270–285        | Aliphatic amines, NO         | 535–560        |
| Imides                 | 170–178        | Aryl                         | 804–913        |
| Imines                 | 310–359        |                              |                |

## Saturated cyclic systems

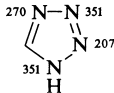
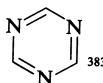
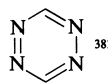
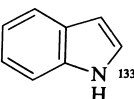
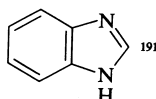
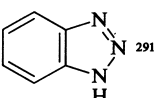
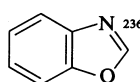
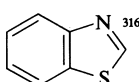
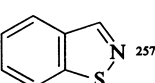
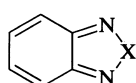
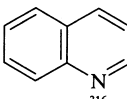
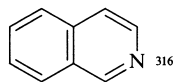
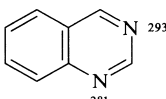
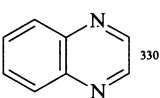
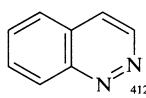
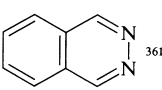
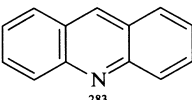
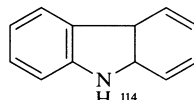
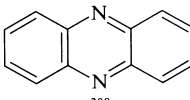
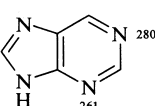
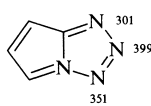
|                                                                                                                                                                         |                                                 |                                                                                                                                                                                                      |                                                                                                         |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
| <br>$(\text{CH}_2)_n\text{—NH}$<br>$n = 2$<br>$n = 3$<br>$n = 4$<br>$n = 5$             | <p>–8.5</p> <p>25.3</p> <p>36.7</p> <p>37.7</p> | <br><br><i>cis</i><br><i>trans</i> | <p>7.5<br/>(in C<sub>6</sub>H<sub>6</sub>)<br/>18.0<br/>(in H<sub>2</sub>O)</p> <p>42.4</p> <p>52.9</p> |
| <br> | <p>32.1</p> <p>35.5</p>                         |                                                                                                                                                                                                      |                                                                                                         |

## Unsaturated cyclic systems

|                                                                                                                                          |                                                                                                       |                                                                                                       |                                                                                                       |
|------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| <br><sup>145</sup>                                     | <br><sup>245</sup> | <br><sup>205</sup> | <br><sup>240</sup> |
| <br><sup>316</sup><br><sup>316</sup><br><sup>244</sup> | <br><sup>251</sup> | <br><sup>383</sup> | <br><sup>323</sup> |



**TABLE 7.63** Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*Continued*)

| Unsaturated cyclic systems (continued)                                             |                                                                                     |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|---|----------------|---|-----|---|-----|----|-----|
|    |    |                                                                                  |  |   |                |   |     |   |     |    |     |
|    |    |                                                                                  |  |   |                |   |     |   |     |    |     |
|    |    | <table><tr><th>X</th><th><math>\delta</math>, ppm</th></tr><tr><td>O</td><td>517</td></tr><tr><td>S</td><td>331</td></tr><tr><td>Se</td><td>373</td></tr></table> |                                                                                   | X | $\delta$ , ppm | O | 517 | S | 331 | Se | 373 |
| X                                                                                  | $\delta$ , ppm                                                                      |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |
| O                                                                                  | 517                                                                                 |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |
| S                                                                                  | 331                                                                                 |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |
| Se                                                                                 | 373                                                                                 |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |
|    |    |                                                                                  |                                                                                   |   |                |   |     |   |     |    |     |
|    |    |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |
|    |    |                                                                                  |                                                                                   |   |                |   |     |   |     |    |     |
|   |   |                                                                                 |                                                                                   |   |                |   |     |   |     |    |     |
|  |  |                                                                               |                                                                                   |   |                |   |     |   |     |    |     |
|  |  |                                                                                                                                                                   |                                                                                   |   |                |   |     |   |     |    |     |

**TABLE 7.64** Nitrogen-15 Chemical Shifts in Monosubstituted Pyridine

$$\delta = 317.3 + \Delta_i$$

| Substituent                          | $\Delta_{C-2}$ | $\Delta_{C-3}$ | $\Delta_{C-4}$ |
|--------------------------------------|----------------|----------------|----------------|
| —CH <sub>3</sub>                     | −0.4           | 0.3            | −8.0           |
| —CH <sub>2</sub> CH <sub>3</sub>     | −1.8           |                | −6.6           |
| —CH(CH <sub>3</sub> ) <sub>2</sub>   | −5.1           |                | −5.9           |
| —C(CH <sub>3</sub> ) <sub>3</sub>    | −2.5           |                | −5.8           |
| —CN                                  | −0.9           | −0.8           | 10.6           |
| —CHO                                 | 10             | 11             | 29             |
| —CO—CH <sub>3</sub>                  | −9             | 15             | 11             |
| —CO—OCH <sub>2</sub> CH <sub>3</sub> | 11.8           |                | −5             |
| —OCH <sub>3</sub>                    | −49            | 0              | −23            |
| —OH                                  | −126           | −2             | −118           |
| —NO <sub>2</sub>                     | −23            | 1              | 22             |
| —NH <sub>2</sub>                     | −45            | 10             | −46            |
| —F                                   | −42            | −18            |                |
| —Cl                                  | −4             | 4              | −6             |
| —Br                                  | 2              | 8              | 7              |

**TABLE 7.65** Nitrogen-15 Chemical Shifts for Standards

Values given in ppm, relative to NH<sub>3</sub> liquid at 23°C.

| Substance                                                                    | $\delta$ , ppm | Conditions                                        |
|------------------------------------------------------------------------------|----------------|---------------------------------------------------|
| Nitromethane (neat)                                                          | 380.2          | For organic solvents and acidic aqueous solutions |
| Potassium (or sodium) nitrate (saturated aqueous solution)                   | 376.5          | For neutral and basic aqueous solutions           |
| C(NO <sub>2</sub> ) <sub>4</sub>                                             | 331            | For nitro compounds                               |
| (CH <sub>3</sub> ) <sub>2</sub> —CHO (neat)                                  | 103.8          | For organic solvents and aqueous solutions        |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> N <sup>+</sup> Cl <sup>−</sup> | 64.4           | Saturated aqueous solution                        |
| (CH <sub>3</sub> ) <sub>4</sub> N <sup>+</sup> Cl <sup>−</sup>               | 43.5           | Saturated aqueous solution                        |
| NH <sub>4</sub> Cl                                                           | 27.3           | Saturated aqueous solution                        |
| NH <sub>4</sub> NO <sub>3</sub>                                              | 20.7           | Saturated aqueous solution                        |
| NH <sub>3</sub>                                                              | 0.0            | Liquid, 25°C                                      |
|                                                                              | −15.9          | Vapor, 5 atm                                      |

**TABLE 7.66** Nitrogen-15 to Hydrogen-1 Spin Coupling Constants

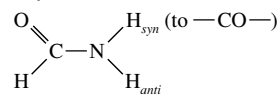
| Structure                                        | $J$ , Hz | Structure                                                                                     | $J$ , Hz |
|--------------------------------------------------|----------|-----------------------------------------------------------------------------------------------|----------|
| R—NH <sub>2</sub> and R <sub>2</sub> NH          | 61–67    | Aryl—NHNH <sub>2</sub>                                                                        | 90       |
| Aryl—NH <sub>2</sub>                             | 78       | <i>p</i> -O <sub>2</sub> N—aryl—NHNH <sub>2</sub>                                             | 99       |
| <i>p</i> -CH <sub>3</sub> O—aryl—NH <sub>2</sub> | 79       | Aryl—SO <sub>2</sub> —NH <sub>2</sub>                                                         | 81       |
| <i>p</i> -O <sub>2</sub> N—aryl—NH <sub>2</sub>  | 90–93    | Aryl—SO <sub>2</sub> —NHR                                                                     | 86       |
| Amine salts (alkyl and aryl)                     | 73–76    |  (to —CO—) | 88       |
| Aryl—NHOH                                        | 79       |                                                                                               |          |
| Aryl—NHCH <sub>3</sub>                           | 87       |                                                                                               |          |
| Aryl—NHCH <sub>2</sub> F                         | 90       |                                                                                               | 92–93    |

TABLE 7.66 Nitrogen-15 to Hydrogen-1 Spin Coupling Constants (Continued)

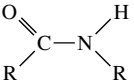
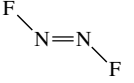
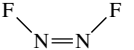
| Structure                                                                        | <i>J</i> , Hz | Structure                            | <i>J</i> , Hz |
|----------------------------------------------------------------------------------|---------------|--------------------------------------|---------------|
|  | 88–92         | (R <sub>3</sub> Si) <sub>2</sub> NH  | 67            |
| Pyrrole                                                                          | 97            | CF <sub>3</sub> —S—NH <sub>2</sub>   | 81            |
| HC≡NH <sup>+</sup>                                                               | 133–136       | (CF <sub>3</sub> —S) <sub>2</sub> NH | 99            |
| ≡P—NH <sub>2</sub>                                                               | 82–90         | Pyridinium ion                       | 90            |
|                                                                                  |               | Quinolinium ion                      | 96            |

TABLE 7.67 Nitrogen-15 to Carbon-13 Spin Coupling Constants

| Structure                           | <i>J</i> , Hz | Structure                                                              | <i>J</i> , Hz |
|-------------------------------------|---------------|------------------------------------------------------------------------|---------------|
| Alkyl amines                        | 4–4.5         | Alkyl—NO <sub>2</sub>                                                  | 11            |
| Cyclic alkyl amines                 | 2–2.5         | R—CN                                                                   | 18            |
| Alkyl amines protonated             | 4–5           | CH <sub>3</sub> — $\overset{\cdot\cdot}{\text{N}}\equiv\bar{\text{C}}$ |               |
| Aryl amines                         | 10–14         | H <sub>3</sub> C—N                                                     | 10            |
| Aryl amines protonated              | 9             | —N≡C                                                                   | 9             |
| CH <sub>3</sub> CO—NH <sub>2</sub>  | 14–15         | Diaryl azoxy                                                           |               |
| H <sub>2</sub> N—CO—NH <sub>2</sub> | 20            | <i>anti</i>                                                            | 18            |
| Aryl—NO <sub>2</sub>                | 15            | <i>syn</i>                                                             | 13            |

TABLE 7.68 Nitrogen-15 to Fluorine-19 Spin Coupling Constants

| Structure                                                                                                        | <i>J</i> , Hz | Structure      | <i>J</i> , Hz |
|------------------------------------------------------------------------------------------------------------------|---------------|----------------|---------------|
| NF <sub>3</sub>                                                                                                  | 155           | Pyridine       |               |
| F <sub>4</sub> N <sub>2</sub>                                                                                    | 164           | 2-F            | 52            |
| FNO <sub>2</sub>                                                                                                 | 158           | 3-F            | 4             |
| F <sub>3</sub> NO                                                                                                | 190           | 2,6-di-F       | 37            |
| F <sub>3</sub> C—O—NF <sub>2</sub>                                                                               | 164–176       | Pyridinium ion |               |
| FCO—NF <sub>2</sub>                                                                                              | 221           | 2-F            | 23            |
| (NF <sub>4</sub> ) <sup>+</sup> SbF <sub>6</sub> <sup>−</sup>                                                    | 323           | 3-F            | 3             |
| (NF <sub>4</sub> ) <sup>+</sup> AsF <sub>6</sub> <sup>−</sup>                                                    | 328           | Quinoline, 8-F | 3             |
| (N <sub>2</sub> F) <sup>+</sup> AsF <sub>6</sub> <sup>−</sup>                                                    | 459           | Aniline        |               |
| F <sub>3</sub> C—NO <sub>2</sub>                                                                                 | 215           | 2-F            | 0             |
|  ( <i>trans</i> <i>J</i> = 10) | 190           | 3-F            | 0             |
|                                                                                                                  |               | 4-F            | 1.5           |
|  ( <i>cis</i> <i>J</i> = 52)   | 203           | Anilinium ion  |               |
|                                                                                                                  |               | 2-F            | 1.4           |
|                                                                                                                  |               | 3-F            | 0.2           |
|                                                                                                                  |               | 4-F            | 0             |

**TABLE 7.69** Fluorine-19 Chemical ShiftsValues given in ppm on the  $\delta$  scale, relative to  $\text{CCl}_3\text{F}$ .

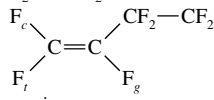
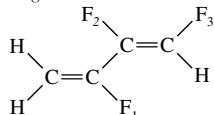
| Substituent group                                                                               | $\delta$ , ppm              | Substituent group                                                                                                                       | $\delta$ , ppm       |
|-------------------------------------------------------------------------------------------------|-----------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|----------------------|
| $-\text{SO}_2-\text{F}$                                                                         | -67 to -42                  | Cyclohexane-F                                                                                                                           | 210                  |
| $-\text{CO}-\text{F}$                                                                           | (aryl)(alkyl)<br>-29 to -20 |                                                                                                                                         | (axial)<br>to<br>240 |
| $>\text{N}-\text{CO}-\text{F}$                                                                  | -5                          |                                                                                                                                         | (equatorial)         |
| Aryl- $\text{CF}_2\text{Cl}$                                                                    | 49                          | Perfluorocycloalkane                                                                                                                    | 131-138              |
| $-\text{CF}_3\text{I}$                                                                          | 56                          | $>\text{CF}-\text{CF}_3$                                                                                                                | 163-198              |
| $-\text{CF}_2\text{Br}$                                                                         | 63                          | $>\text{CF}(\text{CF}_3)_2$                                                                                                             | 180-191              |
| $\text{R}-\text{CF}_2\text{Cl}$                                                                 | 61-71                       | $-\text{CFH}-$                                                                                                                          | 198-231              |
| $>\text{C}-\text{CF}_3$ and aryl- $\text{CF}_3$                                                 | 56-73                       | $-\text{CFH}_2$                                                                                                                         | 235-244              |
| $-\text{CS}-\text{CF}_3$                                                                        | 70                          | $\text{F}_2\text{C}=\text{CF}_2$                                                                                                        | 133                  |
| $>\text{CF}-\text{CF}_3$                                                                        | 71-73                       | $\text{F}_c \quad \text{CF}_2-\text{CF}_2\text{H}$<br> |                      |
| $-\text{S}-\text{CF}_3$                                                                         | 41                          | <i>cis</i>                                                                                                                              | 108                  |
| $-\text{S}-\text{CF}_2-\text{S}-$                                                               | 39                          | <i>trans</i>                                                                                                                            | 92                   |
| $>\text{P}-\text{CF}_3$                                                                         | 46-66                       | <i>gem</i>                                                                                                                              | 192                  |
| $>\text{N}-\text{CF}_3$                                                                         | 40-58                       |                                                        |                      |
| $>\text{N}-\text{CF}_2-\text{C}$                                                                | 85-127                      | F-1                                                                                                                                     | 126                  |
| $-\text{O}-\text{CF}_2-\text{R}$                                                                | 70-91                       | F-2                                                                                                                                     | 155                  |
| $-\text{O}-\text{CF}_2-\text{CF}_3$                                                             | 70-91                       | F-3                                                                                                                                     | 162                  |
| $-\text{CH}_2-\text{CF}_3$                                                                      | 76-77                       | $\text{ClFC}=\text{CH}-\text{CF}_3$                                                                                                     | 61                   |
| $\text{HO}-\text{CO}-\text{CF}_3$                                                               | 77                          | Cycloalkenes                                                                                                                            |                      |
| $-\text{CHF}-\text{CF}_3$                                                                       | 81                          | $=\text{CF}-\text{CF}_2-$                                                                                                               |                      |
| $-\text{CF}_2-\text{CF}_3$                                                                      | 78-88                       | $\text{C}(\text{CF}_3 \text{ or } \text{H})-$                                                                                           | 101-113              |
| $-\text{CS}-\text{F}$                                                                           | 81                          | $-\text{CF}_2-\text{CF}_2-$                                                                                                             |                      |
| $\text{CF}_3-\text{C}-\text{N} \leq$                                                            | 84-96                       | $\text{C}(\text{CF}_3 \text{ or } \text{CH}_3)=$                                                                                        | 110-114              |
| $-\text{CO}-\text{CF}_2-\text{CF}_3$                                                            | 83                          | $-\text{CF}_2-\text{CF}_2-\text{CH}=\text{}$                                                                                            | 113-116              |
| $-\text{CF}_2-$                                                                                 | 86-126                      | $-\text{CF}_2-\text{CF}_2-\text{CF}=\text{}$                                                                                            | 119-122              |
| $-\text{CF}_2\text{Br}$                                                                         | 91                          | Aryl-F                                                                                                                                  | 113                  |
| $-\text{C}-\text{CF}_2-\text{S}-$                                                               | 91-98                       | $\text{C}_{10}\text{H}_7-\text{F}$                                                                                                      |                      |
| $-\text{CF}=\text{}$                                                                            | 180-192                     | F-1                                                                                                                                     | 127                  |
| $-\text{CF}_2-\text{CF}_3$                                                                      | 111                         | F-2                                                                                                                                     | 114                  |
| $-\text{CO}-\text{CF}_2-$                                                                       | 116-131                     | $\text{C}_6\text{H}_5-\text{C}_6\text{H}_4-\text{F}$                                                                                    |                      |
| $-\text{C}(\text{halide})-\text{CF}_2-$                                                         | 119-128                     | F-2                                                                                                                                     | 117                  |
| $-\text{CF}_2-\text{CF}_3$                                                                      | 121-125                     | F-3                                                                                                                                     | 113                  |
| $-\text{CF}_2-\text{CF}_2-$                                                                     | 121-129                     | F-4                                                                                                                                     | 109                  |
| $-\text{CF}_2-\text{CH}_2-$                                                                     | 122-133                     | $\text{C}_6\text{F}_6$                                                                                                                  | 163                  |
| $-\text{CF}_2-\text{CHF}_2$                                                                     | 128-132                     |                                                                                                                                         |                      |
| $-\text{CF}_2\text{H}$                                                                          | 136-143                     |                                                                                                                                         |                      |
|  $\text{F}_2$ | 151-156                     |                                                                                                                                         |                      |
|  $\text{F}_2$ | 147                         |                                                                                                                                         |                      |
|  $\text{F}_2$ | 96-133                      |                                                                                                                                         |                      |
|  $\text{F}$   | 159                         |                                                                                                                                         |                      |

TABLE 7.70 Fluorine-19 Chemical Shifts for Standards

| Substance                                | Formula                           | $\delta$ , ppm |
|------------------------------------------|-----------------------------------|----------------|
| Trichlorofluoromethane                   | $\text{CFCl}_3$                   | 0.0            |
| $\alpha,\alpha,\alpha$ -Trifluorotoluene | $\text{C}_6\text{H}_5\text{CF}_3$ | 63.8           |
| Trifluoroacetic acid                     | $\text{CF}_3\text{COOH}$          | 76.5           |
| Carbon tetrafluoride                     | $\text{CF}_4$                     | 76.7           |
| Fluorobenzene                            | $\text{C}_6\text{H}_5\text{F}$    | 113.1          |
| Perfluorocyclobutane                     | $\text{C}_4\text{F}_8$            | 138.0          |

TABLE 7.71 Fluorine-19 to Fluorine-19 Spin Coupling Constants

| Structure                                                                                 | $J_{\text{FF}}$ , Hz |
|-------------------------------------------------------------------------------------------|----------------------|
| $\text{F}_2\text{C} \begin{array}{c} \diagup \\ \diagdown \end{array} \text{cycloalkane}$ |                      |
| <i>gem</i>                                                                                | 212–260              |
| Unsaturated compounds $\text{>C=C<}$                                                      |                      |
| <i>gem</i>                                                                                | 30–90                |
| <i>trans</i>                                                                              | 115–130              |
| <i>cis</i>                                                                                | 9–58                 |
| Aromatic compounds, monocyclic                                                            |                      |
| <i>ortho</i>                                                                              | 18–22                |
| <i>meta</i>                                                                               | 0–7                  |
| <i>para</i>                                                                               | 12–15                |
| Alkanes                                                                                   |                      |
| $\text{CFCl}_2\text{—CF}_2\text{—CFCl}_2$                                                 | 6                    |
| $\text{CFCl}_2\text{—CF}_2\text{—CCl}_3$                                                  | 5                    |
| $\text{CF}_2\text{Cl—CF}_2\text{—CF}_2\text{Cl}$                                          | 1                    |
| $\text{CF}_3\text{—CF}_2\text{—CF}_2\text{Cl}$ (or $\text{—CF}_3$ )                       | <1                   |
| $\text{CF}_3\text{—CF}_2\text{—CF}_2\text{Cl}$                                            | 2                    |
| $\text{CF}_3\text{—CF}_2\text{—CF}_2\text{Cl}$                                            | 9                    |
| $\text{CF}_3\text{—CF}_2\text{—CF}_3$                                                     | 7                    |

TABLE 7.72 Silicon-29 Chemical Shifts

Values given in ppm on the  $\delta$  scale relative to tetramethylsilane.

| Substituent group X in $(\text{CH}_3)_{4-n}\text{SiX}_n$ | $n$   |          |            |            |
|----------------------------------------------------------|-------|----------|------------|------------|
|                                                          | 1     | 2        | 3          | 4          |
| —F                                                       | 35    | 9        | –52        | –109       |
| —Cl                                                      | 30    | 32       | 13         | –19        |
| —Br                                                      | 26    | 20       | –18        | –94        |
| —I                                                       | 9     | –34      | –18        | –346       |
| —H                                                       | –19   | –42      | –65        | –93        |
| —C <sub>2</sub> H <sub>5</sub>                           | 2     | 5        | 7          | 8          |
| —C <sub>6</sub> H <sub>5</sub>                           | –5    | –9       | –12        |            |
| —CH=CH <sub>2</sub>                                      | –7    | –14      | –21        | –23        |
| —Oalkyl                                                  | 14–17 | –3 to –6 | –41 to –45 | –79 to –83 |
| —Oaryl                                                   | 17    | –6       | –54        | –101       |
| —O—CO—alkyl                                              | 22    | 4        | –43        | –75        |
| —N(CH <sub>3</sub> ) <sub>2</sub>                        | 6     | –2       | –18        | –28        |

**TABLE 7.72** Silicon-29 Chemical Shifts (*Continued*)

| Structure                                                                                                  | $\delta$ , ppm | Structure                                                                                     | $\delta$ , ppm |
|------------------------------------------------------------------------------------------------------------|----------------|-----------------------------------------------------------------------------------------------|----------------|
| <b>Hydrides</b>                                                                                            |                |                                                                                               |                |
| $\text{H}_3\text{Si}-$                                                                                     | -39 to -60     | $\begin{array}{c} \text{O}- \\   \\ \text{CH}_3\text{Si}-\text{O}- \end{array}$ (branching)   | -65 to -66     |
| $- \text{H}_2\text{Si}-$                                                                                   | -5 to -37      | $\begin{array}{c} \text{O}- \\   \\ -\text{O}-\text{Si}-\text{O}- \end{array}$ (cross-linked) | -105 to -110   |
| $\text{HSi} \leq$                                                                                          | -2 to -39      | $\begin{array}{c} \text{O}- \\   \\ \text{O}- \end{array}$                                    |                |
| <b>Silicates</b>                                                                                           |                | <b>Polysilanes</b>                                                                            |                |
| Orthosilicate anions                                                                                       | -69 to -72     | $\text{F}_3\text{Si}-\text{SiF}_3$                                                            | -74            |
| Silicon in end position                                                                                    | -77 to -81     | $\text{Cl}_3\text{Si}-\text{SiCl}_3$                                                          | -8             |
| Silicon in middle                                                                                          | -85 to -89     | $(\text{CH}_3\text{O})_3\text{Si}-\text{Si}(\text{OCH}_3)_3$                                  | -53            |
| Branching silicons                                                                                         | -93 to -97     | $(\text{CH}_3)_3\text{Si}-\text{Si}(\text{CH}_3)_3$                                           | -20            |
| Cross-linked silicons                                                                                      | -107 to -120   | $(\text{CH}_3)_2\text{Si}[\text{Si}(\text{CH}_3)_3]_2$                                        | -48            |
| <b>Methyl siloxanes</b>                                                                                    |                | $\text{HSi}[\text{Si}(\text{CH}_3)_3]_3$                                                      | -117           |
| $(\text{CH}_3)_2\text{Si}-\text{O}-$ (end position)                                                        | 6-8            | $\text{Si}[\text{Si}(\text{CH}_3)_3]_4$                                                       | -135           |
| $\begin{array}{c} \text{O}- \\   \\ (\text{CH}_3)_2\text{Si} \end{array}$ (middle)                         | -18 to -23     |                                                                                               |                |
| $\begin{array}{c} \text{O}- \\   \\ \text{O}- \\   \\ \text{CH}_3\text{Si}(\text{H}) \end{array}$ (middle) | -35 to -36     |                                                                                               |                |

**TABLE 7.73** Phosphorus-31 Chemical Shifts

Values given in ppm on the  $\delta$  scale, relative to 85%  $\text{H}_3\text{PO}_4$ .

| Structure                        | Identical atoms attached directly to phosphorus | Non-identically substituted phosphorus |                            |                            |
|----------------------------------|-------------------------------------------------|----------------------------------------|----------------------------|----------------------------|
|                                  |                                                 | R = $\text{CH}_3$                      | R = $\text{C}_2\text{H}_5$ | R = $\text{C}_6\text{H}_5$ |
| $\text{P}_4$                     | 461                                             |                                        |                            |                            |
| $\text{PR}_3$                    |                                                 | 62                                     | 20                         | 6                          |
| $\text{PHR}_2$                   |                                                 | 99                                     | 56                         | 41                         |
| $\text{PH}_2\text{R}$            |                                                 | 164                                    | 128                        | 122                        |
| $\text{PH}_3$                    | 241                                             |                                        |                            |                            |
| $\text{PF}_3$                    | -97                                             |                                        |                            |                            |
| $\text{PRF}_2$                   |                                                 |                                        | -168                       | -207                       |
| $\text{PCl}_3$                   | -220                                            |                                        |                            |                            |
| $\text{PRCl}_2$                  |                                                 | -192                                   | -196                       | -162                       |
| $\text{PR}_2\text{Cl}$           |                                                 | -94                                    | -119                       | -81                        |
| $\text{PBr}_3$                   | -227                                            |                                        |                            |                            |
| $\text{PRBr}_2$                  |                                                 | -184                                   | -194                       | -152                       |
| $\text{PR}_2\text{Br}$           |                                                 | -91                                    | -116                       | -71                        |
| $\text{PI}_3$                    | -178                                            |                                        |                            |                            |
| $\text{P}(\text{CN})_3$          | 136                                             |                                        |                            |                            |
| $\text{P}(\text{SiR}_3)_3$       |                                                 | 251                                    |                            |                            |
| $\text{P}(\text{OR})_3$          |                                                 | -141                                   | -139                       | -127                       |
| $\text{P}(\text{OR})_2\text{Cl}$ |                                                 | -169                                   | -165                       | -157                       |
| $\text{P}(\text{OR})\text{Cl}_2$ |                                                 | -114                                   | -177                       | -173                       |
| $\text{P}(\text{SR})_3$          |                                                 | -125                                   | -115                       | -132                       |
| $\text{P}(\text{SR})_2\text{Cl}$ |                                                 | -188                                   | -186                       | -183                       |
| $\text{P}(\text{SR})\text{Cl}_2$ |                                                 | -206                                   | -211                       | -204                       |
| $\text{P}(\text{SR})_2\text{Br}$ |                                                 |                                        |                            | -184                       |

**TABLE 7.73** Phosphorus-31 Chemical Shifts (*Continued*)

| Structure                          | Identical atoms attached directly to phosphorus | Non-identically substituted phosphorus |                                   |                                   |
|------------------------------------|-------------------------------------------------|----------------------------------------|-----------------------------------|-----------------------------------|
|                                    |                                                 | R = CH <sub>3</sub>                    | R = C <sub>2</sub> H <sub>5</sub> | R = C <sub>6</sub> H <sub>5</sub> |
| P(SR)Br <sub>2</sub>               |                                                 | −204                                   |                                   |                                   |
| P(NR <sub>2</sub> ) <sub>3</sub>   |                                                 | −123                                   | −118                              |                                   |
| P(NR <sub>2</sub> )Cl <sub>2</sub> |                                                 | −166                                   | −162                              | −151                              |
| PR(NR <sub>2</sub> ) <sub>2</sub>  |                                                 | −86                                    | −100                              | −100                              |
| PR <sub>2</sub> (NR <sub>2</sub> ) |                                                 | −39                                    | −62                               |                                   |
| F <sub>2</sub> P—PF <sub>2</sub>   | −226                                            |                                        |                                   |                                   |
| Cl <sub>2</sub> P—PCl <sub>2</sub> | −155                                            |                                        |                                   |                                   |
| I <sub>2</sub> P—PI <sub>2</sub>   | −170                                            |                                        |                                   |                                   |
| PH <sub>2</sub> ·K <sup>+</sup>    | 255                                             |                                        |                                   |                                   |
| P(CF <sub>3</sub> ) <sub>3</sub>   | 3                                               |                                        |                                   |                                   |
| P <sub>4</sub> O <sub>6</sub>      | −113                                            |                                        |                                   |                                   |

| Structure             | Identical atoms attached directly to phosphorus | Non-identically substituted phosphorus |        |        |
|-----------------------|-------------------------------------------------|----------------------------------------|--------|--------|
|                       |                                                 | X = F                                  | X = Cl | X = Br |
| P(NCO) <sub>3</sub>   | −97                                             |                                        |        |        |
| P(NCO) <sub>2</sub> X |                                                 | −128                                   | −128   | −127   |
| P(NCO)X <sub>2</sub>  |                                                 | −131                                   | −166   |        |
| P(NCS) <sub>3</sub>   | −86                                             |                                        |        |        |
| P(NCS) <sub>2</sub> X |                                                 |                                        | −114   | −112   |
| P(NCS)X <sub>2</sub>  |                                                 |                                        | −155   | −153   |

| Structure                                           | Identical atoms attached directly to phosphorus | Non-identically substituted phosphorus |                                   |                                   |
|-----------------------------------------------------|-------------------------------------------------|----------------------------------------|-----------------------------------|-----------------------------------|
|                                                     |                                                 | R = CH <sub>3</sub>                    | R = C <sub>2</sub> H <sub>5</sub> | R = C <sub>6</sub> H <sub>5</sub> |
| O=PR <sub>3</sub>                                   |                                                 | −36                                    | −48                               | −25                               |
| O=PHR <sub>2</sub>                                  |                                                 | −63                                    |                                   | −23                               |
| O=PF <sub>3</sub>                                   | 36                                              |                                        |                                   |                                   |
| O=PRF <sub>2</sub>                                  |                                                 | −27                                    | −29                               | −11                               |
| O=PCl <sub>3</sub>                                  | −2                                              |                                        |                                   |                                   |
| O=PRCl <sub>2</sub>                                 |                                                 | −45                                    | −53                               | −34                               |
| O=PR <sub>2</sub> Cl                                |                                                 | −65                                    | −77                               | −43                               |
| O=P(OR) <sub>3</sub>                                |                                                 | −1                                     | 1                                 | 18                                |
| O=P(OR) <sub>2</sub> Cl                             |                                                 | −6                                     | −3                                | 6                                 |
| O=P(OR)Cl <sub>2</sub>                              |                                                 | −6                                     | −6                                | −2                                |
| O=PH(OR) <sub>2</sub>                               |                                                 | −19                                    | −15                               |                                   |
| O=PR <sub>2</sub> (OC <sub>2</sub> H <sub>5</sub> ) |                                                 | −50                                    | −52                               | −31                               |
| O=PR(OC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>  |                                                 | −30                                    | −33                               | −17                               |
| O=P(NR <sub>2</sub> ) <sub>3</sub>                  |                                                 | −23                                    | −24                               | −2                                |
| O=PR <sub>2</sub> (NR <sub>2</sub> )                |                                                 | −44                                    |                                   | −26                               |
| O=P(OR) <sub>2</sub> NH <sub>2</sub>                |                                                 | −15                                    | −12                               | −3                                |
| O=P(OR) <sub>2</sub> (NCS)                          |                                                 |                                        | 19                                | 29                                |
| O=P(SR) <sub>3</sub>                                |                                                 | −66                                    | −61                               | −55                               |
| O=PBr <sub>3</sub>                                  | 103                                             |                                        |                                   |                                   |
| O=P(NCO) <sub>3</sub>                               | 41                                              |                                        |                                   |                                   |
| O=P(NCS) <sub>3</sub>                               | 62                                              |                                        |                                   |                                   |
| O=P(NH <sub>2</sub> ) <sub>3</sub>                  | −22                                             |                                        |                                   |                                   |

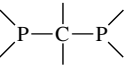
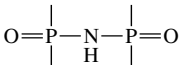
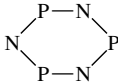
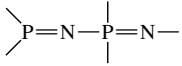
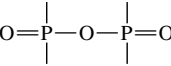
**TABLE 7.73** Phosphorus-31 Chemical Shifts (*Continued*)

| Structure                                             | Identical atoms attached directly to phosphorus | Structure                                                                                                                                 | Identical atoms attached directly to phosphorus |                                   |  |
|-------------------------------------------------------|-------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|-----------------------------------|--|
| PF <sub>5</sub>                                       | 35                                              | $\begin{array}{c} \text{O} \\   \\ -\text{O}-\text{P}-\text{O}- \\   \\ \text{OR} \\ \text{(middle group)} \end{array}$                   | ca 18                                           |                                   |  |
| PF <sub>6</sub> <sup>-</sup> H <sup>+</sup>           | 144                                             |                                                                                                                                           |                                                 |                                   |  |
| PBr <sub>5</sub>                                      | 101                                             |                                                                                                                                           |                                                 |                                   |  |
| P(OC <sub>2</sub> H <sub>5</sub> ) <sub>5</sub>       | 71                                              |                                                                                                                                           |                                                 |                                   |  |
| PO <sub>4</sub> <sup>3-</sup>                         | -6                                              | $\begin{array}{c} \text{O} \\   \\ -\text{O}-\text{P}-\text{O}- \\   \\ \text{O} \\ \text{P (etc.)} \\ \text{(branch group)} \end{array}$ | ca 30                                           |                                   |  |
| O=P[OSi(CH <sub>3</sub> ) <sub>3</sub> ] <sub>3</sub> | 33                                              |                                                                                                                                           |                                                 |                                   |  |
| H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>          | 11                                              |                                                                                                                                           |                                                 |                                   |  |
| Phosphonates                                          | -24 to -2                                       |                                                                                                                                           |                                                 |                                   |  |
| Phosphonium cations                                   |                                                 |                                                                                                                                           |                                                 |                                   |  |
| Alkyl                                                 | -43 to -32                                      |                                                                                                                                           |                                                 |                                   |  |
| Aryl                                                  | -35 to -18                                      |                                                                                                                                           |                                                 |                                   |  |
| (O <sub>3</sub> P—PO <sub>3</sub> ) <sup>4-</sup>     | -9                                              |                                                                                                                                           |                                                 |                                   |  |
| Polyphosphates                                        |                                                 |                                                                                                                                           |                                                 |                                   |  |
| O=P—O—<br> <br>(OR) <sub>2</sub><br>(end group)       | ca 6                                            |                                                                                                                                           |                                                 |                                   |  |
| Structure                                             | Identical atoms attached directly to phosphorus | Non-identically substituted phosphorus                                                                                                    |                                                 |                                   |  |
|                                                       |                                                 | R = CH <sub>3</sub>                                                                                                                       | R = C <sub>2</sub> H <sub>5</sub>               | R = C <sub>6</sub> H <sub>5</sub> |  |
| S=PR <sub>3</sub>                                     | -29                                             | -59                                                                                                                                       | -55                                             | -43                               |  |
| S=PCl <sub>3</sub>                                    |                                                 |                                                                                                                                           |                                                 |                                   |  |
| S=PRCl <sub>2</sub>                                   |                                                 | -80                                                                                                                                       | -94                                             | -75                               |  |
| S=PR <sub>2</sub> Cl                                  |                                                 | -87                                                                                                                                       | -109                                            | -80                               |  |
| S=PBr <sub>3</sub>                                    | 112                                             |                                                                                                                                           |                                                 |                                   |  |
| S=PRBr <sub>2</sub>                                   |                                                 | -21                                                                                                                                       | -42                                             | -20                               |  |
| S=PR <sub>2</sub> Br                                  |                                                 | -64                                                                                                                                       | -98                                             |                                   |  |
| S=P(OR) <sub>3</sub>                                  |                                                 | -73                                                                                                                                       | -68                                             | -53                               |  |
| S=P(OR)Cl <sub>2</sub>                                |                                                 | -59                                                                                                                                       | -56                                             | -54                               |  |
| S=P(OR) <sub>2</sub> Cl                               |                                                 | -73                                                                                                                                       | -68                                             | -59                               |  |
| S=PH(OR) <sub>2</sub>                                 |                                                 | -74                                                                                                                                       | -69                                             | -59                               |  |
| S=P(SR) <sub>3</sub>                                  |                                                 | -98                                                                                                                                       | -92                                             | -92                               |  |
| S=P(NH <sub>2</sub> ) <sub>3</sub>                    | -60                                             |                                                                                                                                           |                                                 |                                   |  |
| S=P(NR <sub>2</sub> ) <sub>3</sub>                    |                                                 | -82                                                                                                                                       | -78                                             |                                   |  |
| Se=P(OR) <sub>3</sub>                                 |                                                 | -78                                                                                                                                       | -71                                             | -58                               |  |
| Se=P(SR) <sub>3</sub>                                 |                                                 | -82                                                                                                                                       | -76                                             |                                   |  |
| P(OR) <sub>5</sub>                                    |                                                 |                                                                                                                                           | 71                                              | 86                                |  |
| PRF <sub>4</sub>                                      |                                                 | 30                                                                                                                                        | 30                                              | 42                                |  |
| PR <sub>2</sub> F <sub>3</sub>                        |                                                 | -9                                                                                                                                        | -6                                              |                                   |  |



**TABLE 7.74** Phosphorus-31 Spin Coupling Constants[illegible]

**TABLE 7.74** Phosphorus-31 Spin Coupling Constants (*Continued*)

| Substituent group                                                                | $J_{\text{pp}}$ , Hz | Substituent group                                                                 | $J_{\text{pp}}$ , Hz |
|----------------------------------------------------------------------------------|----------------------|-----------------------------------------------------------------------------------|----------------------|
|  | ca 70                |  | 8–30                 |
| $\text{>P-O-P<}$                                                                 | 20–40                |  | 5–66                 |
| $\text{>P-S-P<}$                                                                 | 86–90                |  | 5–65                 |
|  | 15–25                |                                                                                   |                      |

## 7.8 MASS SPECTROMETRY

### 7.8.1 Correlation of Mass Spectra with Molecular Structure

**7.8.1.1 Molecular Identification.** In the identification of a compound, the most important information is the molecular weight. The mass spectrometer is able to provide this information, often to four decimal places. One assumes that no ions heavier than the molecular ion form when using electron-impact ionization. The chemical ionization spectrum will often show a cluster around the nominal molecular weight.

Several relationships aid in deducing the empirical formula of the parent ion (and also molecular fragments). From the empirical formula hypothetical molecular structures can be proposed, using the entries in the formula indices of Beilstein and *Chemical Abstracts*.

**7.8.1.2 Natural Isotopic Abundances.** The relative abundances of natural isotopes produce peaks one or more mass units larger than the parent ion (Table 7.75a). For a compound  $\text{C}_w\text{H}_x\text{O}_z\text{N}_y$ , a formula allows one to calculate the percent of the heavy isotope contributions from a monoisotopic peak,  $P_M$ , to the  $P_{M+1}$  peak:

$$100 \frac{P_{M+1}}{P_M} = 0.015x + 1.11w + 0.37y + 0.037z$$

Tables of abundance factors have been calculated for all combinations of C, H, N, and O up to mass 500 (J. H. Beynon and A. E. Williams, *Mass and Abundance Tables for Use in Mass Spectrometry*, Elsevier, Amsterdam, 1963).

Compounds that contain chlorine, bromine, sulfur, or silicon are usually apparent from prominent peaks at masses 2, 4, 6, and so on, units larger than the nominal mass of the parent or fragment ion. For example, when one chlorine atom is present, the  $P + 2$  mass peak will be about one-third the intensity of the parent peak. When one bromine atom is present, the  $P + 2$  mass peak will be about the same intensity as the parent peak. The abundance of heavy isotopes is treated in terms of the binomial expansion  $(a + b)^m$ , where  $a$  is the relative abundance of the light isotope,  $b$  is the relative abundance of the heavy isotope, and  $m$  is the number of atoms of the particular element present in the molecule. If two bromine atoms are present, the binomial expansion is

$$(a + b)^2 = a^2 + 2ab + b^2$$

TABLE 7.75 Isotopic Abundances and Masses of Selected Elements

| (a) Abundances of some polyisotopic elements, % |           |                  |           |                  |           |
|-------------------------------------------------|-----------|------------------|-----------|------------------|-----------|
| Element                                         | Abundance | Element          | Abundance | Element          | Abundance |
| <sup>1</sup> H                                  | 99.985    | <sup>16</sup> O  | 99.76     | <sup>33</sup> S  | 0.76      |
| <sup>2</sup> H                                  | 0.015     | <sup>17</sup> O  | 0.037     | <sup>34</sup> S  | 4.22      |
| <sup>12</sup> C                                 | 98.892    | <sup>18</sup> O  | 0.204     | <sup>35</sup> Cl | 75.53     |
| <sup>13</sup> C                                 | 1.108     | <sup>28</sup> Si | 92.18     | <sup>37</sup> Cl | 24.47     |
| <sup>14</sup> N                                 | 99.63     | <sup>29</sup> Si | 4.71      | <sup>79</sup> Br | 50.52     |
| <sup>15</sup> N                                 | 0.37      | <sup>30</sup> Si | 3.12      | <sup>81</sup> Br | 49.48     |

| (b) Selected isotope masses |         |                  |          |
|-----------------------------|---------|------------------|----------|
| Element                     | Mass    | Element          | Mass     |
| <sup>1</sup> H              | 1.0078  | <sup>31</sup> P  | 30.9738  |
| <sup>12</sup> C             | 12.0000 | <sup>32</sup> S  | 31.9721  |
| <sup>14</sup> N             | 14.0031 | <sup>35</sup> Cl | 34.9689  |
| <sup>16</sup> O             | 15.9949 | <sup>56</sup> Fe | 55.9349  |
| <sup>19</sup> F             | 18.9984 | <sup>79</sup> Br | 78.9184  |
| <sup>28</sup> Si            | 27.9769 | <sup>127</sup> I | 126.9047 |

Now substituting the percent abundance of each isotope (<sup>79</sup>Br and <sup>81</sup>Br) into the expansion,

$$(0.505)^2 + 2(0.505)(0.495) + (0.495)^2$$

gives 
$$0.255 + 0.500 + 0.250$$

which are the proportions of  $P:(P + 2):(P + 4)$ , a triplet that is slightly distorted from a 1:2:1 pattern. When two elements with heavy isotopes are present, the binomial expansion  $(a + b)^m(c + d)^n$  is used.

Sulfur-34 enhances the  $P + 2$  peak by 4.2%; silicon-29 enhances the  $P + 1$  peak by 4.7% and the  $P + 2$  peak by 3.1%.

**7.8.1.3 Exact Mass Differences.** If the exact mass of the parent or fragment ions are ascertained with a high-resolution mass spectrometer, this relationship is often useful for combinations of C, H, N, and O (Table 7.75b):

$$\frac{\text{Exact mass difference from nearest integral mass} + 0.0051z - 0.0031y}{0.0078} = \text{number of hydrogens}$$

One substitutes integral numbers (guesses) for  $z$  (oxygen) and  $y$  (nitrogen) until the divisor becomes an integral multiple of the numerator within 0.0002 mass unit.

For example, if the exact mass is 177.0426 for a compound containing only C, H, O, and N (note the odd mass which indicates an odd number of nitrogen atoms), then

$$\frac{0.0426 + 0.0051z - 0.0031y}{0.0078} = 7 \text{ hydrogen atoms}$$

when  $z = 3$  and  $y = 1$ . The empirical formula is  $\text{C}_9\text{H}_7\text{NO}_3$  since

$$\frac{177 - 7(1) - 1(14) - 3(16)}{12} = 9 \text{ carbon atoms}$$

**7.8.1.4 Number of Rings and Double Bonds.** The total number of rings and double bonds can be determined from the empirical formula ( $\text{C}_w\text{H}_x\text{O}_z\text{N}_y$ ) by the relationship

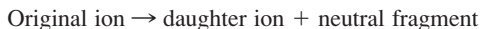
$$\frac{1}{2(2w - x + y + z)}$$

when covalent bonds comprise the molecular structure. Remember the total number for a benzene ring is four (one ring and three double bonds); a triple bond has two.

### 7.8.1.5 General Rules

1. If the nominal molecular weight of a compound containing only C, H, O, and N is even, so is the number of hydrogen atoms it contains.
2. If the nominal molecular weight is divisible by four, the number of hydrogen atoms is also divisible by four.
3. When the nominal molecular weight of a compound containing only C, H, O, and N is odd, the number of nitrogen atoms must be odd.

**7.8.1.6 Metastable Peaks.** If the mass spectrometer has a field-free region between the exit of the ion source and the entrance to the mass analyzer, metastable peaks  $m^*$  may appear as a weak, diffuse (often humped-shape) peak, usually at a nonintegral mass. The one-step decomposition process takes the general form:



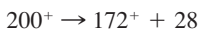
The relationship between the original ion and daughter ion is given by

$$m^* = \frac{(\text{mass of daughter ion})^2}{\text{mass of original ion}}$$

For example, a metastable peak appeared at 147.9 mass units in a mass spectrum with prominent peaks at 65, 91, 92, 107, 108, 155, 172, and 200 mass units. Try all possible combinations in the above expression. The fit is given by

$$147.9 = \frac{(172)^2}{200}$$

which provides this information:



The probable neutral fragment lost is either  $\text{CH}_2=\text{CH}_2$  or CO.

### 7.8.2 Mass Spectra and Structure

The mass spectrum is a fingerprint for each compound because no two molecules are fragmented and ionized in exactly the same manner on electron-impact ionization. In reporting mass spectra the data are normalized by assigning the most intense peak (denoted as base peak) a value of 100. Other peaks are reported as percentages of the base peak.

A very good general survey for interpreting mass spectral data is given by R. M. Silverstein, G. C. Bassler, and T. C. Morrill, *Spectrometric Identification of Organic Compounds*, 4th ed., Wiley, New York, 1981.

#### 7.8.2.1 Initial Steps in Elucidation of a Mass Spectrum

1. Tabulate the prominent ion peaks, starting with the highest mass.
2. Usually only one bond is cleaved. In succeeding fragmentations a new bond is formed for each additional bond that is broken.
3. When fragmentation is accompanied by the formation of a new bond as well as by the breaking of an existing bond, a rearrangement process is involved. These will be even mass peaks when only C, H, and O are involved. The migrating atom is almost exclusively hydrogen; six-membered cyclic transition states are most important.
4. Tabulate the probable groups that (a) give rise to the prominent charged ion peaks and (b) list the neutral fragments.

#### 7.8.2.2 General Rules for Fragmentation Patterns

1. Bond cleavage is more probable at branched carbon atoms: tertiary > secondary > primary. The positive charge tends to remain with the branched carbon.
2. Double bonds favor cleavage beta to the carbon (but see rule 6).
3. A strong parent peak often indicates a ring.
4. Saturated ring systems lose side chains at the alpha carbon. Upon fragmentation, two ring atoms are usually lost.
5. A heteroatom induces cleavage at the bond beta to it.
6. Compounds that contain a carbonyl group tend to break at this group; the positive charge remains with the carbonyl portion.
7. For linear alkanes, the initial fragment lost is an ethyl group (never a methyl group), followed by propyl, butyl, and so on. An intense peak at mass 43 suggests a chain longer than butane.
8. The presence of Cl, Br, S, and Si can be deduced from the unusual isotopic abundance patterns of these elements. These elements can be traced through the positively charged fragments until the pattern disappears or changes due to the loss of one of these atoms to a neutral fragment.
9. When unusual mass differences occur between some fragments ions, the presence of F (mass difference 19), I (mass difference 127), or P (mass difference 31) should be suspected.

#### 7.8.2.3 Characteristic Low-Mass Fragment Ions

Mass 30 = Primary amines

Masses 31, 45, 59 = Alcohol or ether

Masses 19 and 31 = Alcohol

Mass 66 = Monobasic carboxylic acid

Masses 77 and 91 = Benzene ring

#### 7.8.2.4 Characteristic Low-Mass Neutral Fragments from the Molecular Ion

Mass 18 ( $\text{H}_2\text{O}$ ) = From alcohols, aldehydes, ketones

Mass 19 (F) and 20 (HF) = Fluorides

Mass 27 (HCN) = Aromatic nitriles or nitrogen heterocycles

Mass 29 = Indicates either CHO or  $\text{C}_2\text{H}_5$

Mass 30 = Indicates either  $\text{CH}_2\text{O}$  or NO

Mass 33 (HS) and 34 ( $\text{H}_2\text{S}$ ) = Thiols

Mass 42 =  $\text{CH}_2\text{CO}$  via rearrangement from a methyl ketone or an aromatic acetate or an aryl- $\text{NHCOCH}_3$  group

Mass 43 =  $\text{C}_3\text{H}_7$  or  $\text{CH}_3\text{CO}$

Mass 45 =  $\text{COOH}$  or  $\text{OC}_2\text{H}_5$

Table 7.76 is condensed, with permission, from the Catalog of Mass Spectral Data of the American Petroleum Institute Research Project 44. These, and other tables, should be consulted for further and more detailed information.

Included in the table are all compounds for which information was available through the  $\text{C}_7$  compounds. The mass number for the five most important peaks for each compound are listed, followed in each case by the relative intensity in parentheses. The intensities in all cases are normalized to the *n*-butane 43 peak taken as 100. Another method for expressing relative intensities is to assign the base peak a value of 100 and express the relative intensities of the other peaks as a ratio to the base peak. Taking ethyl nitrate as an example, the tabulated values would be

|               |             |         |          |          |          |
|---------------|-------------|---------|----------|----------|----------|
| Ethyl nitrate | 91(0.01)(P) | 46(100) | 29(44.2) | 30(30.5) | 76(24.2) |
|---------------|-------------|---------|----------|----------|----------|

The compounds are arranged in the table according to their molecular formulas. Each formula is arranged alphabetically, except that C is first if carbon occurs in the molecules, followed by H if it occurs. The formulas are then arranged alphabetically and according to increasing number of atoms of each kind, all  $\text{C}_4$  compounds being listed before any  $\text{C}_5$  compounds, and so on.

Nearly all these spectra have been recorded using 70-V electrons to bombard the sample molecules.

TABLE 7.76 Condensed Table of Mass Spectra

| Molecular<br>formula                          | Name                              | Mass numbers (and intensities) of: |              |                               |          |          |
|-----------------------------------------------|-----------------------------------|------------------------------------|--------------|-------------------------------|----------|----------|
|                                               |                                   | Parent<br>peak                     | Base<br>peak | Three next most intense peaks |          |          |
| B <sub>2</sub> H <sub>6</sub>                 | Diborane                          | 28(0.13)                           | 26(54)       | 27(52)                        | 24(48)   | 25(30)   |
| B <sub>3</sub> H <sub>6</sub> N <sub>3</sub>  | Triborine triamine                | 81(21)                             | 80(58)       | 79(37)                        | 53(29)   | 52(22)   |
| B <sub>3</sub> H <sub>9</sub>                 | Pentaborane                       | 64(15)                             | 59(30)       | 60(30)                        | 62(24)   | 61(21)   |
| CBrClF <sub>2</sub>                           | Diffuorochlorobromomethane        | 164(0.23)                          | 85(86)       | 87(27)                        | 129(17)  | 131(16)  |
| CBr <sub>2</sub> F <sub>2</sub>               | Diffuorodibromomethane            | 208(1.7)                           | 129(70)      | 131(68)                       | 79(18)   | 31(18)   |
| CCl <sub>2</sub> F <sub>2</sub>               | Diffuorodichloromethane           | 120(0.07)                          | 85(33)       | 87(11)                        | 50(3.9)  | 101(2.8) |
| CCl <sub>3</sub> F                            | Fluorotrichloromethane            | 136(0.04)                          | 101(54)      | 103(35)                       | 66(7.0)  | 35(5.8)  |
| CCl <sub>4</sub>                              | Tetrachloromethane                | 152(0.0)                           | 117(39)      | 119(37)                       | 35(16)   | 47(16)   |
| CF <sub>3</sub> I                             | Trifluoroiodomethane              | 196(51)                            | 196(51)      | 127(49)                       | 69(40)   | 177(16)  |
| CF <sub>4</sub>                               | Tetrafluoromethane                | 88(0.0)                            | 69(57)       | 50(6.8)                       | 19(3.9)  | 31(2.8)  |
| CHBrClF                                       | Fluorochlorobromomethane          | 148(5.5)                           | 67(120)      | 69(38)                        | 31(13)   | 111(11)  |
| CHBrF <sub>2</sub>                            | Diffuorobromomethane              | 130(13)                            | 51(83)       | 31(18)                        | 132(13)  | 79(13)   |
| CHCl <sub>3</sub>                             | Trichloromethane                  | 118(1.3)                           | 83(69)       | 85(44)                        | 47(24)   | 35(13)   |
| CHF <sub>3</sub>                              | Trifluoromethane                  | 70(0.25)                           | 69(20)       | 51(18)                        | 31(9.9)  | 50(2.9)  |
| CHN                                           | Hydrogen cyanide                  | 27(92)                             | 27(92)       | 26(15)                        | 12(3.8)  | 28(1.6)  |
| CH <sub>2</sub> ClF                           | Fluorochloromethane               | 68(48)                             | 68(48)       | 33(25)                        | 70(15)   | 49(11)   |
| CH <sub>2</sub> Cl <sub>2</sub>               | Dichloromethane                   | 84(41)                             | 49(71)       | 86(26)                        | 51(21)   | 47(13)   |
| CH <sub>2</sub> F <sub>2</sub>                | Diffuoromethane                   | 52(2.7)                            | 33(26)       | 51(25)                        | 31(7.3)  | 32(2.9)  |
| CH <sub>2</sub> O                             | Methanal (formaldehyde)           | 30(19)                             | 29(21)       | 28(6.6)                       | 14(0.94) | 13(0.92) |
| CH <sub>3</sub> O <sub>2</sub>                | Methanoic acid (formic)           | 46(72)                             | 29(118)      | 45(56)                        | 28(20)   | 17(20)   |
| CH <sub>3</sub> Cl                            | Chloromethane                     | 50(66)                             | 50(66)       | 15(54)                        | 52(21)   | 49(6.6)  |
| CH <sub>3</sub> F                             | Monofluoromethane                 | 34(29)                             | 15(31)       | 33(28)                        | 14(5.3)  | 31(3.2)  |
| CH <sub>3</sub> I                             | Iodomethane                       | 142(78)                            | 142(78)      | 127(29)                       | 141(11)  | 15(10)   |
| CH <sub>3</sub> NO <sub>2</sub>               | Nitromethane                      | 61(35)                             | 30(65)       | 15(34)                        | 46(23)   | 29(5.3)  |
| CH <sub>4</sub>                               | Methane                           | 16(67)                             | 16(67)       | 15(58)                        | 14(11)   | 13(5.5)  |
| CH <sub>4</sub> O                             | Methanol                          | 32(26)                             | 31(38)       | 29(25)                        | 28(2.4)  | 18(0.7)  |
| CH <sub>4</sub> S                             | Methanethiol                      | 48(49)                             | 47(65)       | 45(40)                        | 46(9.5)  | 15(8.9)  |
| CH <sub>5</sub> N                             | Aminomethane (methylamine)        | 31(30)                             | 30(53)       | 28(47)                        | 29(8.7)  | 27(8.6)  |
| CO                                            | Carbon monoxide                   | 28(78)                             | 28(78)       | 12(3.7)                       | 16(1.3)  | 29(0.9)  |
| COS                                           | Carbonyl sulfide                  | 60(83)                             | 60(83)       | 32(48)                        | 28(6.9)  | 12(5.0)  |
| CO <sub>2</sub>                               | Carbon dioxide                    | 44(76)                             | 44(76)       | 28(5.0)                       | 16(4.7)  | 12(1.9)  |
| CS <sub>2</sub>                               | Carbon disulfide                  | 76(184)                            | 76(184)      | 32(40)                        | 44(33)   | 78(16)   |
| C <sub>2</sub> F <sub>4</sub>                 | Tetrafluoroethene                 | 100(20)                            | 31(47)       | 81(34)                        | 50(14)   | 12(3.6)  |
| C <sub>2</sub> F <sub>6</sub>                 | Hexafluoroethane                  | 138(0.14)                          | 69(95)       | 119(39)                       | 31(17)   | 50(9.6)  |
| C <sub>2</sub> F <sub>5</sub> Hg              | Hexafluorodimethylmercury         | 340(0.83)                          | 69(111)      | 202(26)                       | 271(22)  | 200(21)  |
| C <sub>2</sub> H <sub>2</sub>                 | Ethyne                            | 26(102)                            | 26(102)      | 25(20)                        | 24(5.7)  | 13(5.7)  |
| C <sub>2</sub> H <sub>2</sub> CIN             | Chloroethanenitrile               | 75(51)                             | 75(51)       | 48(46)                        | 40(23)   | 77(16)   |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> | <i>cis</i> -1,2-Dichloroethene    | 96(53)                             | 61(72)       | 98(34)                        | 63(23)   | 26(22)   |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> | <i>trans</i> -1,2,-Dichloroethene | 96(49)                             | 61(73)       | 98(32)                        | 26(25)   | 63(23)   |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub> | 1,1,2,2-Tetrachloroethane         | 166(5.9)                           | 83(95)       | 85(60)                        | 95(11)   | 87(9.7)  |
| C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>  | 1,1-Difluoroethene                | 64(32)                             | 64(32)       | 45(21)                        | 31(16)   | 33(13)   |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> | 1,1,1-Trichloroethane             | 132(0.0)                           | 97(37)       | 99(24)                        | 61(19)   | 117(7.1) |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> | 1,1,2-Trichloroethane             | 132(3.9)                           | 97(43)       | 83(41)                        | 99(27)   | 85(26)   |
| C <sub>2</sub> H <sub>3</sub> F <sub>3</sub>  | 1,1,1-Trifluoroethane             | 84(0.94)                           | 69(81)       | 65(31)                        | 15(13)   | 45(10)   |
| C <sub>2</sub> H <sub>3</sub> N               | Ethanenitrile                     | 41(89)                             | 41(89)       | 40(46)                        | 39(17)   | 38(10)   |
| C <sub>2</sub> H <sub>4</sub>                 | Ethene (ethylene)                 | 28(66)                             | 28(66)       | 27(43)                        | 26(41)   | 25(7.8)  |
| C <sub>2</sub> H <sub>4</sub> BrCl            | 1-Chloro-2-bromoethane            | 142(7.9)                           | 63(93)       | 27(82)                        | 65(30)   | 26(24)   |
| C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub> | 1,2-Dibromoethane                 | 186(1.6)                           | 27(93)       | 107(72)                       | 109(67)  | 26(23)   |
| C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> | 1,1-Dichloroethane                | 98(5.7)                            | 63(89)       | 27(64)                        | 65(28)   | 26(21)   |

**TABLE 7.76** Condensed Table of Mass Spectra (*Continued*)

| Molecular formula                              | Name                       | Mass numbers (and intensities) of: |           |                               |         |         |
|------------------------------------------------|----------------------------|------------------------------------|-----------|-------------------------------|---------|---------|
|                                                |                            | Parent peak                        | Base peak | Three next most intense peaks |         |         |
| C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>  | 1,2-Dichloroethane         | 98(1.7)                            | 62(12)    | 27(11)                        | 49(4.9) | 64(3.9) |
| C <sub>2</sub> H <sub>4</sub> N <sub>2</sub>   | Diazoethane                | 56(16)                             | 28(27)    | 27(25)                        | 26(21)  | 41(5.2) |
| C <sub>2</sub> H <sub>4</sub> O                | Ethanal (acetaldehyde)     | 44(30)                             | 29(66)    | 43(18)                        | 42(6.1) | 26(6.1) |
| C <sub>2</sub> H <sub>4</sub> O                | Ethylene oxide             | 44(30)                             | 29(46)    | 15(30)                        | 14(12)  | 43(7.1) |
| C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>   | Ethanoic acid (acetic)     | 60(19)                             | 43(37)    | 45(33)                        | 15(21)  | 14(8.0) |
| C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>   | Methyl formate             | 60(27)                             | 31(96)    | 29(60)                        | 32(33)  | 28(6.8) |
| C <sub>2</sub> H <sub>5</sub> Br               | Bromoethane                | 108(35)                            | 29(54)    | 27(48)                        | 110(33) | 26(16)  |
| C <sub>2</sub> H <sub>5</sub> Cl               | Chloroethane               | 64(36)                             | 64(36)    | 28(32)                        | 29(30)  | 27(27)  |
| C <sub>2</sub> H <sub>5</sub> F                | Fluoroethane               | 48(2.4)                            | 47(24)    | 27(8.9)                       | 33(8.2) | 26(3.0) |
| C <sub>2</sub> H <sub>5</sub> N                | Ethylenimine               | 43(31)                             | 42(56)    | 28(44)                        | 15(20)  | 41(11)  |
| C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>  | Nitroethane                | 75(0.0)                            | 29(85)    | 27(74)                        | 30(19)  | 26(11)  |
| C <sub>2</sub> H <sub>5</sub> NO <sub>3</sub>  | Ethyl nitrate              | 91(0.01)                           | 46(95)    | 29(42)                        | 30(29)  | 76(23)  |
| C <sub>2</sub> H <sub>6</sub>                  | Ethane                     | 30(26)                             | 28(99)    | 27(33)                        | 26(23)  | 29(21)  |
| C <sub>2</sub> H <sub>6</sub> O                | Ethanol                    | 46(9.7)                            | 31(63)    | 45(22)                        | 29(14)  | 27(14)  |
| C <sub>2</sub> H <sub>6</sub> O                | Dimethyl ether             | 46(32)                             | 45(71)    | 29(56)                        | 15(41)  | 14(8.9) |
| C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>   | Dimethyl peroxide          | 62(28)                             | 29(47)    | 31(45)                        | 15(16)  | 30(12)  |
| C <sub>2</sub> H <sub>6</sub> S                | 2-Thiopropane              | 62(56)                             | 47(69)    | 45(42)                        | 46(29)  | 35(24)  |
| C <sub>2</sub> H <sub>6</sub> S                | Ethanethiol                | 62(44)                             | 62(44)    | 29(43)                        | 47(36)  | 27(35)  |
| C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>   | 2,3-Dithiabutane           | 94(95)                             | 94(95)    | 45(59)                        | 79(56)  | 46(34)  |
| C <sub>2</sub> H <sub>6</sub> S <sub>3</sub>   | 2,3,4-Trithiapentane       | 126(54)                            | 126(54)   | 45(32)                        | 79(27)  | 47(19)  |
| C <sub>2</sub> H <sub>7</sub> N                | Aminoethane (ethylamine)   | 45(18)                             | 30(96)    | 28(28)                        | 44(19)  | 27(13)  |
| C <sub>2</sub> H <sub>7</sub> N                | N-Methylaminomethane       | 45(36)                             | 44(71)    | 28(48)                        | 15(14)  | 42(13)  |
| C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>   | 1,2-Diaminoethane          | 60(2.7)                            | 30(111)   | 18(14)                        | 42(6.9) | 43(5.9) |
| C <sub>3</sub> F <sub>6</sub>                  | Hexafluoropropene          | 150(16)                            | 31(56)    | 69(44)                        | 131(41) | 100(20) |
| C <sub>3</sub> F <sub>8</sub>                  | Octafluoropropane          | 188(0.0)                           | 69(171)   | 31(49)                        | 169(42) | 50(16)  |
| C <sub>3</sub> H <sub>3</sub> N                | Propenenitrile             | 53(55)                             | 26(55)    | 52(41)                        | 51(18)  | 27(10)  |
| C <sub>3</sub> H <sub>4</sub>                  | Propadiene                 | 40(72)                             | 40(72)    | 39(69)                        | 38(29)  | 37(23)  |
| C <sub>3</sub> H <sub>4</sub>                  | Propyne (methylacetylene)  | 40(79)                             | 40(79)    | 39(73)                        | 38(29)  | 37(22)  |
| C <sub>3</sub> H <sub>4</sub> ClN              | 3-Chloropropanenitrile     | 89(12)                             | 49(68)    | 54(54)                        | 51(29)  | 26(20)  |
| C <sub>3</sub> H <sub>4</sub> O                | Propenal (acrolein)        | 56(16)                             | 27(25)    | 26(15)                        | 28(13)  | 55(11)  |
| C <sub>3</sub> H <sub>5</sub> Cl               | 1-Chloro-1-propene         | 76(30)                             | 41(70)    | 39(43)                        | 40(10)  | 78(9.6) |
| C <sub>3</sub> H <sub>5</sub> ClO              | 3-Chloro-1,2-epoxypropane  | 92(0.19)                           | 57(55)    | 27(53)                        | 29(40)  | 31(21)  |
| C <sub>3</sub> H <sub>5</sub> ClO <sub>2</sub> | Methyl chloroacetate       | 109(0.23)                          | 59(56)    | 49(44)                        | 15(43)  | 29(37)  |
| C <sub>3</sub> H <sub>5</sub> Cl <sub>3</sub>  | 1,2,3-Trichloropropane     | 146(0.71)                          | 75(61)    | 110(22)                       | 77(19)  | 61(18)  |
| C <sub>3</sub> H <sub>5</sub> N                | Propanenitrile             | 55(8.3)                            | 28(83)    | 54(51)                        | 26(17)  | 27(15)  |
| C <sub>3</sub> H <sub>6</sub>                  | Cyclopropane               | 42(64)                             | 42(64)    | 41(58)                        | 39(44)  | 27(23)  |
| C <sub>3</sub> H <sub>6</sub>                  | Propene                    | 42(39)                             | 41(58)    | 39(41)                        | 27(22)  | 40(17)  |
| C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub>  | 1,1-Dichloropropane        | 112(0.0)                           | 63(27)    | 41(25)                        | 77(22)  | 62(19)  |
| C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub>  | 1,2-Dichloropropane        | 112(2.6)                           | 63(51)    | 62(36)                        | 27(29)  | 41(25)  |
| C <sub>3</sub> H <sub>6</sub> O                | 1-Propen-3-ol (allyl alc.) | 58(12)                             | 57(43)    | 29(34)                        | 31(26)  | 27(19)  |
| C <sub>3</sub> H <sub>6</sub> O                | Propanal                   | 58(25)                             | 29(66)    | 28(46)                        | 27(38)  | 26(14)  |
| C <sub>3</sub> H <sub>6</sub> O                | Propanone (acetone)        | 58(24)                             | 43(85)    | 15(26)                        | 27(5.9) | 42(5.9) |
| C <sub>3</sub> H <sub>6</sub> O                | 1,2-Epoxypropane           | 58(19)                             | 28(44)    | 29(30)                        | 27(28)  | 26(18)  |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>   | 1,3-Dioxolane              | 74(3.1)                            | 73(52)    | 43(36)                        | 44(30)  | 29(30)  |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>   | Propanoic acid             | 74(27)                             | 28(34)    | 29(28)                        | 27(21)  | 45(19)  |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>   | Ethyl formate              | 74(5.8)                            | 31(82)    | 28(60)                        | 29(54)  | 27(36)  |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>   | Methyl acetate             | 74(22)                             | 43(148)   | 29(16)                        | 42(15)  | 59(8.4) |
| C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>   | Methyl carbonate           | 90(3.3)                            | 15(93)    | 45(54)                        | 29(43)  | 31(34)  |
| C <sub>3</sub> H <sub>7</sub> Br               | 1-Bromopropane             | 122(14)                            | 43(94)    | 27(55)                        | 41(47)  | 39(22)  |



TABLE 7.76 Condensed Table of Mass Spectra (Continued)

| Molecular<br>formula                                         | Name                               | Mass numbers (and intensities) of: |              |                               |         |         |
|--------------------------------------------------------------|------------------------------------|------------------------------------|--------------|-------------------------------|---------|---------|
|                                                              |                                    | Parent<br>peak                     | Base<br>peak | Three next most intense peaks |         |         |
| C <sub>3</sub> H <sub>7</sub> Br                             | 2-Bromopropane                     | 122(11)                            | 43(100)      | 27(50)                        | 41(47)  | 39(24)  |
| C <sub>3</sub> H <sub>7</sub> Cl                             | 1-Chloropropane                    | 78(3.6)                            | 42(60)       | 29(27)                        | 27(22)  | 41(14)  |
| C <sub>3</sub> H <sub>7</sub> Cl                             | 2-Chloropropane                    | 78(14)                             | 43(58)       | 27(20)                        | 63(15)  | 41(13)  |
| C <sub>3</sub> H <sub>7</sub> F                              | 2-Fluoropropane                    | 62(1.0)                            | 47(84)       | 46(24)                        | 61(12)  | 27(7.6) |
| C <sub>3</sub> H <sub>7</sub> N                              | 2-Methylethylenimine               | 57(22)                             | 28(76)       | 56(34)                        | 30(24)  | 29(19)  |
| C <sub>3</sub> H <sub>7</sub> N                              | <i>N</i> -Methylethylenimine       | 57(31)                             | 42(94)       | 15(46)                        | 28(25)  | 27(17)  |
| C <sub>3</sub> H <sub>7</sub> NO                             | <i>N,N</i> -Dimethylformamide      | 73(54)                             | 44(63)       | 42(29)                        | 28(25)  | 15(24)  |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>                | 1-Nitropropane                     | 89(0.0)                            | 43(68)       | 27(67)                        | 41(58)  | 39(24)  |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>                | 2-Nitropropane                     | 89(0.0)                            | 43(75)       | 41(55)                        | 27(53)  | 39(23)  |
| C <sub>3</sub> H <sub>8</sub>                                | Propane                            | 44(25)                             | 29(85)       | 28(50)                        | 27(33)  | 43(19)  |
| C <sub>3</sub> H <sub>8</sub> O                              | 1-Propanol                         | 60(7.2)                            | 31(115)      | 27(18)                        | 29(17)  | 59(10)  |
| C <sub>3</sub> H <sub>8</sub> O                              | 2-Propanol                         | 60(0.45)                           | 45(112)      | 43(19)                        | 27(18)  | 29(11)  |
| C <sub>3</sub> H <sub>8</sub> O                              | Methyl ethyl ether                 | 60(24)                             | 45(94)       | 29(46)                        | 15(23)  | 27(19)  |
| C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                 | Dimethoxymethane                   | 76(1.6)                            | 45(117)      | 29(51)                        | 75(51)  | 15(48)  |
| C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                 | 2-Methoxy-1-ethanol                | 76(7.3)                            | 45(122)      | 29(44)                        | 15(38)  | 31(32)  |
| C <sub>3</sub> H <sub>8</sub> S                              | 2-Thiabutane                       | 76(47)                             | 61(73)       | 48(40)                        | 47(30)  | 27(27)  |
| C <sub>3</sub> H <sub>8</sub> S                              | 1-Propanethiol                     | 76(30)                             | 47(43)       | 43(34)                        | 27(34)  | 41(32)  |
| C <sub>3</sub> H <sub>8</sub> S                              | 2-Propanethiol                     | 76(41)                             | 43(65)       | 41(44)                        | 27(41)  | 61(26)  |
| C <sub>3</sub> H <sub>9</sub> N                              | 1-Aminopropane                     | 59(1.5)                            | 30(20)       | 28(2.5)                       | 27(1.3) | 41(1.0) |
| C <sub>3</sub> H <sub>9</sub> N                              | Trimethylamine                     | 59(37)                             | 58(95)       | 42(44)                        | 15(32)  | 30(17)  |
| C <sub>3</sub> H <sub>12</sub> B <sub>3</sub> N <sub>3</sub> | <i>B,B',B''</i> -Trimethylborazole | 123(30)                            | 108(102)     | 107(77)                       | 67(38)  | 66(34)  |
| C <sub>4</sub> F <sub>6</sub>                                | Hexafluorocyclobutene              | 162(21)                            | 93(80)       | 31(51)                        | 143(15) | 74(6.9) |
| C <sub>4</sub> F <sub>6</sub>                                | Hexafluoro-1,3-butadiene           | 162(27)                            | 93(90)       | 31(45)                        | 74(10)  | 112(10) |
| C <sub>4</sub> F <sub>6</sub>                                | Hexafluoro-2-butyne                | 162(18)                            | 93(47)       | 143(38)                       | 31(25)  | 69(20)  |
| C <sub>4</sub> F <sub>8</sub>                                | Octafluorocyclobutane              | 200(0.12)                          | 100(97)      | 131(84)                       | 31(53)  | 69(24)  |
| C <sub>4</sub> F <sub>8</sub>                                | Octafluoromethylpropene            | 200(14)                            | 69(74)       | 181(54)                       | 31(44)  | 93(22)  |
| C <sub>4</sub> F <sub>8</sub>                                | Octafluoro-1-butene                | 200(11)                            | 131(122)     | 31(86)                        | 69(44)  | 93(16)  |
| C <sub>4</sub> F <sub>10</sub>                               | Decafluorobutane                   | 238(0.0)                           | 69(178)      | 119(33)                       | 31(22)  | 100(15) |
| C <sub>4</sub> HF <sub>7</sub> O <sub>2</sub>                | Heptafluorobutanoic acid           | 214(0.0)                           | 45(26)       | 69(24)                        | 119(17) | 100(14) |
| C <sub>4</sub> H <sub>2</sub>                                | 1,3-Butadiyne                      | 50(133)                            | 50(133)      | 49(57)                        | 48(14)  | 25(12)  |
| C <sub>4</sub> H <sub>4</sub>                                | 1-Buten-3-yne                      | 52(55)                             | 52(55)       | 51(28)                        | 50(23)  | 49(7.2) |
| C <sub>4</sub> H <sub>4</sub> O                              | Furan                              | 68(36)                             | 39(58)       | 38(9.7)                       | 29(9.3) | 40(6.7) |
| C <sub>4</sub> H <sub>4</sub> S                              | Thiophene                          | 84(93)                             | 84(93)       | 58(56)                        | 45(49)  | 39(24)  |
| C <sub>4</sub> H <sub>4</sub> S <sub>2</sub>                 | 2-Thiophenethiol                   | 116(68)                            | 116(68)      | 71(64)                        | 45(31)  | 39(11)  |
| C <sub>4</sub> H <sub>5</sub> N                              | 3-Butenenitrile                    | 67(27)                             | 41(80)       | 39(36)                        | 27(30)  | 40(20)  |
| C <sub>4</sub> H <sub>5</sub> N                              | Pyrrrole                           | 67(67)                             | 67(67)       | 39(46)                        | 41(42)  | 40(36)  |
| C <sub>4</sub> H <sub>6</sub>                                | 1,2-Butadiene                      | 54(65)                             | 54(65)       | 27(35)                        | 53(29)  | 39(28)  |
| C <sub>4</sub> H <sub>6</sub>                                | 1,3-Butadiene                      | 54(46)                             | 39(53)       | 27(36)                        | 53(31)  | 28(24)  |
| C <sub>4</sub> H <sub>6</sub>                                | 1-Butyne                           | 54(64)                             | 54(64)       | 39(49)                        | 53(27)  | 27(26)  |
| C <sub>4</sub> H <sub>6</sub>                                | 2-Butyne                           | 54(93)                             | 54(93)       | 27(42)                        | 53(41)  | 39(24)  |
| C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub> | Ethyl dichloroacetate              | 156(0.12)                          | 29(192)      | 27(58)                        | 83(23)  | 28(19)  |
| C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>                 | 2,3-Butanedione                    | 86(13)                             | 43(118)      | 15(40)                        | 14(12)  | 42(8.6) |
| C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>                 | Methyl 2-propenoate                | 86(2.0)                            | 55(98)       | 27(66)                        | 15(27)  | 26(22)  |
| C <sub>4</sub> H <sub>7</sub> BrO <sub>2</sub>               | 2-Bromoethyl acetate               | 166(0.03)                          | 43(158)      | 27(35)                        | 106(31) | 108(30) |
| C <sub>4</sub> H <sub>7</sub> Cl                             | 2-Chloro-2-butene                  | 90(27)                             | 55(68)       | 27(21)                        | 39(21)  | 29(18)  |
| C <sub>4</sub> H <sub>7</sub> ClO <sub>2</sub>               | 2-Chloroethyl acetate              | 122(0.0)                           | 43(162)      | 73(43)                        | 15(36)  | 27(29)  |
| C <sub>4</sub> H <sub>7</sub> ClO <sub>2</sub>               | Ethyl chloroacetate                | 122(0.96)                          | 29(130)      | 27(41)                        | 77(37)  | 49(29)  |
| C <sub>4</sub> H <sub>7</sub> N                              | 2-Methylpropanenitrile             | 69(1.7)                            | 42(79)       | 68(38)                        | 28(26)  | 54(19)  |
| C <sub>4</sub> H <sub>7</sub> N                              | <i>n</i> -Butanenitrile            | 69(0.15)                           | 41(112)      | 29(70)                        | 27(38)  | 28(11)  |

TABLE 7.76 Condensed Table of Mass Spectra (*Continued*)

| Molecular formula                             | Name                            | Mass numbers (and intensities) of: |           |                               |         |         |
|-----------------------------------------------|---------------------------------|------------------------------------|-----------|-------------------------------|---------|---------|
|                                               |                                 | Parent peak                        | Base peak | Three next most intense peaks |         |         |
| C <sub>4</sub> H <sub>8</sub>                 | Cyclobutane                     | 56(41)                             | 28(65)    | 41(58)                        | 27(27)  | 26(15)  |
| C <sub>4</sub> H <sub>8</sub>                 | 2-Methylpropene                 | 56(36)                             | 41(85)    | 39(37)                        | 28(18)  | 27(17)  |
| C <sub>4</sub> H <sub>8</sub>                 | 1-Butene                        | 56(32)                             | 41(87)    | 39(30)                        | 27(26)  | 28(26)  |
| C <sub>4</sub> H <sub>8</sub>                 | <i>cis</i> -2-Butene            | 56(36)                             | 41(76)    | 39(27)                        | 27(25)  | 28(24)  |
| C <sub>4</sub> H <sub>8</sub>                 | <i>trans</i> -2-Butene          | 56(37)                             | 41(80)    | 27(27)                        | 39(26)  | 28(26)  |
| C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> | 1,2-Dichlorobutane              | 126(0.30)                          | 41(39)    | 77(35)                        | 27(20)  | 76(16)  |
| C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> | 1,4-Dichlorobutane              | 126(0.03)                          | 55(87)    | 41(29)                        | 27(24)  | 90(23)  |
| C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> | <i>dl</i> -2,3-Dichlorobutane   | 126(0.95)                          | 63(63)    | 62(58)                        | 27(57)  | 55(29)  |
| C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> | <i>meso</i> -2,3-Dichlorobutane | 126(0.95)                          | 63(64)    | 27(57)                        | 62(54)  | 55(31)  |
| C <sub>4</sub> H <sub>8</sub> N <sub>2</sub>  | Acetaldazine                    | 84(23)                             | 42(92)    | 15(47)                        | 28(46)  | 69(38)  |
| C <sub>4</sub> H <sub>8</sub> O               | Butanal                         | 72(19)                             | 27(41)    | 29(38)                        | 44(34)  | 43(32)  |
| C <sub>4</sub> H <sub>8</sub> O               | 2-Butanone                      | 72(17)                             | 43(97)    | 29(24)                        | 27(15)  | 57(6.0) |
| C <sub>4</sub> H <sub>8</sub> O               | Ethyl ethenyl ether             | 72(27)                             | 44(64)    | 43(56)                        | 29(49)  | 27(43)  |
| C <sub>4</sub> H <sub>8</sub> O               | <i>cis</i> -2,3-Epoxybutane     | 72(3.6)                            | 43(67)    | 44(39)                        | 27(35)  | 29(33)  |
| C <sub>4</sub> H <sub>8</sub> O               | <i>trans</i> -2,3-Epoxybutane   | 72(3.5)                            | 43(69)    | 44(35)                        | 29(32)  | 27(31)  |
| C <sub>4</sub> H <sub>8</sub> O               | Tetrahydrofuran                 | 72(22)                             | 42(76)    | 41(39)                        | 27(25)  | 71(20)  |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | 2-Methyl-1,3-dioxacyclopentane  | 88(0.33)                           | 73(67)    | 43(48)                        | 45(44)  | 29(34)  |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | 1,4-Dioxane                     | 88(42)                             | 28(138)   | 29(51)                        | 58(33)  | 31(24)  |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | 2-Methylpropanoic acid          | 88(8.1)                            | 43(77)    | 41(33)                        | 27(26)  | 73(19)  |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | <i>n</i> -Butanoic acid         | 88(1.0)                            | 60(40)    | 73(12)                        | 27(9.6) | 41(9.1) |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | <i>n</i> -Propyl formate        | 88(0.41)                           | 31(123)   | 42(89)                        | 29(38)  | 27(36)  |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | Ethyl acetate                   | 88(7.1)                            | 43(181)   | 29(46)                        | 45(24)  | 27(24)  |
| C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>  | Methyl propanoate               | 88(23)                             | 29(110)   | 57(83)                        | 27(40)  | 59(27)  |
| C <sub>4</sub> H <sub>8</sub> S               | 3-Methylthiacyclobutane         | 88(42)                             | 46(101)   | 45(31)                        | 39(24)  | 47(21)  |
| C <sub>4</sub> H <sub>8</sub> S               | Thiacyclopentane                | 88(44)                             | 60(82)    | 45(29)                        | 46(29)  | 47(22)  |
| C <sub>4</sub> H <sub>9</sub> Br              | 1-Bromobutane                   | 136(7.0)                           | 57(86)    | 41(63)                        | 29(50)  | 27(46)  |
| C <sub>4</sub> H <sub>9</sub> Br              | 2-Bromobutane                   | 136(0.72)                          | 57(108)   | 41(65)                        | 29(61)  | 27(36)  |
| C <sub>4</sub> H <sub>9</sub> N               | Pyrrolidine                     | 71(24)                             | 43(102)   | 28(38)                        | 70(33)  | 42(20)  |
| C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> | <i>n</i> -Butyl nitrite         | 103(0.0)                           | 27(55)    | 43(54)                        | 41(50)  | 30(47)  |
| C <sub>4</sub> H <sub>10</sub>                | 2-Methylpropane                 | 58(3.2)                            | 43(117)   | 41(45)                        | 42(39)  | 27(33)  |
| C <sub>4</sub> H <sub>10</sub>                | <i>n</i> -Butane                | 58(12)                             | 43(100)   | 29(44)                        | 27(37)  | 28(33)  |
| C <sub>4</sub> H <sub>10</sub> Hg             | Diethylmercury                  | 260(12)                            | 29(188)   | 27(54)                        | 28(21)  | 231(15) |
| C <sub>4</sub> H <sub>10</sub> O              | 2-Methyl-1-propanol             | 74(7.5)                            | 43(84)    | 31(56)                        | 42(48)  | 41(47)  |
| C <sub>4</sub> H <sub>10</sub> O              | 2-Methyl-2-propanol             | 74(0.0)                            | 59(92)    | 31(31)                        | 41(19)  | 43(14)  |
| C <sub>4</sub> H <sub>10</sub> O              | 1-Butanol                       | 74(0.37)                           | 31(52)    | 56(44)                        | 41(31)  | 43(30)  |
| C <sub>4</sub> H <sub>10</sub> O              | 2-Butanol                       | 74(0.30)                           | 45(116)   | 31(23)                        | 59(22)  | 27(20)  |
| C <sub>4</sub> H <sub>10</sub> O              | Diethyl ether                   | 74(22)                             | 31(73)    | 59(34)                        | 29(29)  | 45(28)  |
| C <sub>4</sub> H <sub>10</sub> O              | Methyl isopropyl ether          | 74(8.3)                            | 59(126)   | 29(42)                        | 43(37)  | 15(32)  |
| C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> | 1,1-Dimethoxyethane             | 90(0.06)                           | 59(93)    | 29(52)                        | 15(37)  | 31(37)  |
| C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> | 1,2-Dimethoxyethane             | 90(12)                             | 45(177)   | 29(53)                        | 15(50)  | 60(16)  |
| C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> | 2-Ethoxyethanol                 | 90(0.49)                           | 31(112)   | 29(57)                        | 59(56)  | 27(31)  |
| C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> | Diethyl peroxide                | 90(20)                             | 29(116)   | 15(42)                        | 45(34)  | 62(30)  |
| C <sub>4</sub> H <sub>10</sub> S              | 3-Methyl-2-thiabutane           | 90(41)                             | 41(49)    | 75(47)                        | 43(41)  | 48(38)  |
| C <sub>4</sub> H <sub>10</sub> S              | 2-Thiapentane                   | 90(58)                             | 61(126)   | 48(50)                        | 41(43)  | 27(43)  |
| C <sub>4</sub> H <sub>10</sub> S              | 3-Thiapentane                   | 90(41)                             | 75(59)    | 47(51)                        | 27(39)  | 61(33)  |
| C <sub>4</sub> H <sub>10</sub> S              | 2-Methyl-1-propanethiol         | 90(35)                             | 41(60)    | 43(46)                        | 56(34)  | 47(29)  |
| C <sub>4</sub> H <sub>10</sub> S              | 2-Methyl-2-propanethiol         | 90(34)                             | 41(68)    | 57(61)                        | 29(44)  | 39(21)  |
| C <sub>4</sub> H <sub>10</sub> S              | 1-Butanethiol                   | 90(40)                             | 56(74)    | 41(65)                        | 27(42)  | 47(31)  |
| C <sub>4</sub> H <sub>10</sub> S              | 2-Butanethiol                   | 90(34)                             | 41(56)    | 57(50)                        | 61(46)  | 29(46)  |

TABLE 7.76 Condensed Table of Mass Spectra (Continued)

| Molecular formula                              | Name                                   | Mass numbers (and intensities) of: |           |                               |         |         |
|------------------------------------------------|----------------------------------------|------------------------------------|-----------|-------------------------------|---------|---------|
|                                                |                                        | Parent peak                        | Base peak | Three next most intense peaks |         |         |
| C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>  | 2,3-Dithiahexane                       | 122(37)                            | 80(53)    | 43(36)                        | 41(27)  | 27(25)  |
| C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>  | 3,4-Dithiahexane                       | 122(73)                            | 29(82)    | 66(81)                        | 27(57)  | 94(53)  |
| C <sub>4</sub> H <sub>10</sub> SO <sub>3</sub> | Ethyl sulfite                          | 138(3.3)                           | 29(131)   | 31(59)                        | 45(42)  | 27(39)  |
| C <sub>4</sub> H <sub>11</sub> N               | <i>N</i> -Ethylaminoethane             | 73(17)                             | 58(83)    | 30(81)                        | 28(30)  | 27(24)  |
| C <sub>4</sub> H <sub>11</sub> N               | 1-Amino-2-methylpropane                | 73(1.0)                            | 30(22)    | 28(2.0)                       | 41(1.2) | 27(1.1) |
| C <sub>4</sub> H <sub>11</sub> N               | 2-Amino-2-methylpropane                | 73(0.25)                           | 58(127)   | 41(26)                        | 42(20)  | 15(18)  |
| C <sub>4</sub> H <sub>11</sub> N               | 1-Aminobutane                          | 73(12)                             | 30(200)   | 28(23)                        | 27(16)  | 18(12)  |
| C <sub>4</sub> H <sub>11</sub> N               | 2-Aminobutane                          | 73(1.2)                            | 44(170)   | 18(25)                        | 41(18)  | 58(18)  |
| C <sub>4</sub> H <sub>12</sub> Pb              | Tetramethyllead                        | 268(0.14)                          | 253(69)   | 223(59)                       | 208(46) | 251(36) |
| C <sub>5</sub> F <sub>10</sub>                 | Decafluorocyclopentane                 | 250(0.62)                          | 131(173)  | 100(41)                       | 31(40)  | 69(28)  |
| C <sub>5</sub> F <sub>12</sub>                 | Dodecafluoro-2-methylbutane            | 288(0.0)                           | 69(277)   | 119(45)                       | 131(23) | 31(18)  |
| C <sub>5</sub> F <sub>12</sub>                 | Dodecafluoropentane                    | 288(0.08)                          | 69(259)   | 119(76)                       | 169(25) | 31(24)  |
| C <sub>5</sub> HF <sub>9</sub>                 | Nonafluorocyclopentane                 | 232(0.07)                          | 131(61)   | 113(49)                       | 69(34)  | 31(19)  |
| C <sub>5</sub> H <sub>5</sub> N                | Pyridine                               | 79(135)                            | 79(135)   | 52(95)                        | 51(48)  | 50(35)  |
| C <sub>5</sub> H <sub>6</sub>                  | Cyclopentadiene                        | 66(95)                             | 66(95)    | 65(40)                        | 39(35)  | 40(30)  |
| C <sub>5</sub> H <sub>6</sub>                  | <i>trans</i> -2-Penten-4-yne           | 66(77)                             | 66(77)    | 39(54)                        | 65(38)  | 40(35)  |
| C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>   | 2-Methylpyrazine                       | 94(81)                             | 94(81)    | 67(48)                        | 26(33)  | 39(30)  |
| C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>   | Furfuryl alcohol                       | 98(3.4)                            | 98(3.4)   | 41(3.3)                       | 39(3.3) | 42(2.6) |
| C <sub>5</sub> H <sub>6</sub> S                | 2-Methylthiophene                      | 98(68)                             | 97(125)   | 45(26)                        | 39(17)  | 53(11)  |
| C <sub>5</sub> H <sub>6</sub> S                | 3-Methylthiophene                      | 98(74)                             | 97(138)   | 45(35)                        | 39(14)  | 27(11)  |
| C <sub>5</sub> H <sub>8</sub>                  | Methylenecyclobutane                   | 68(38)                             | 40(67)    | 67(48)                        | 39(47)  | 53(21)  |
| C <sub>5</sub> H <sub>8</sub>                  | Spiropentane                           | 68(8.9)                            | 67(58)    | 40(56)                        | 39(52)  | 53(23)  |
| C <sub>5</sub> H <sub>8</sub>                  | Cyclopentene                           | 68(41)                             | 67(99)    | 39(36)                        | 53(23)  | 41(19)  |
| C <sub>5</sub> H <sub>8</sub>                  | 3-Methyl-1,2-butadiene                 | 68(53)                             | 68(53)    | 53(40)                        | 39(28)  | 41(26)  |
| C <sub>5</sub> H <sub>8</sub>                  | 2-Methyl-1,3-butadiene                 | 68(40)                             | 67(48)    | 53(41)                        | 39(34)  | 27(23)  |
| C <sub>5</sub> H <sub>8</sub>                  | 1,2-Pentadiene                         | 68(39)                             | 68(39)    | 53(38)                        | 39(37)  | 27(31)  |
| C <sub>5</sub> H <sub>8</sub>                  | <i>cis</i> -1,3-Pentadiene             | 68(40)                             | 67(53)    | 39(43)                        | 53(38)  | 41(25)  |
| C <sub>5</sub> H <sub>8</sub>                  | <i>trans</i> -1,3-Pentadiene           | 68(41)                             | 67(52)    | 39(43)                        | 53(39)  | 41(26)  |
| C <sub>5</sub> H <sub>8</sub>                  | 1,4-Pentadiene                         | 68(40)                             | 39(47)    | 67(35)                        | 53(33)  | 41(30)  |
| C <sub>5</sub> H <sub>8</sub>                  | 2,3-Pentadiene                         | 68(62)                             | 68(62)    | 53(42)                        | 39(36)  | 41(31)  |
| C <sub>5</sub> H <sub>8</sub>                  | 3-Methyl-1-butyne                      | 68(8.5)                            | 53(74)    | 67(45)                        | 27(35)  | 39(21)  |
| C <sub>5</sub> H <sub>8</sub>                  | 1-Pentyne                              | 68(8.7)                            | 67(50)    | 40(44)                        | 39(42)  | 27(34)  |
| C <sub>5</sub> H <sub>8</sub>                  | 2-Pentyne                              | 68(67)                             | 68(67)    | 53(61)                        | 39(32)  | 27(27)  |
| C <sub>5</sub> H <sub>8</sub> N <sub>2</sub>   | 3,5-Dimethylpyrazole                   | 96(47)                             | 96(47)    | 95(37)                        | 39(16)  | 54(12)  |
| C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>   | 2,4-Pentanedione                       | 100(22)                            | 43(120)   | 85(33)                        | 15(23)  | 27(11)  |
| C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>   | 2-Propenyl acetate                     | 100(0.16)                          | 43(177)   | 41(30)                        | 39(29)  | 15(28)  |
| C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>   | Methyl methacrylate                    | 100(26)                            | 41(78)    | 69(52)                        | 39(31)  | 15(16)  |
| C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub> | Ethyl 3-chloropropanoate               | 136(0.70)                          | 27(65)    | 29(62)                        | 91(42)  | 63(37)  |
| C <sub>5</sub> H <sub>10</sub>                 | <i>cis</i> -1,2-Dimethylcyclopropane   | 70(39)                             | 55(77)    | 42(35)                        | 39(32)  | 41(32)  |
| C <sub>5</sub> H <sub>10</sub>                 | <i>trans</i> -1,2-Dimethylcyclopropane | 70(42)                             | 55(79)    | 42(34)                        | 41(33)  | 39(30)  |
| C <sub>5</sub> H <sub>10</sub>                 | Ethylcyclopropane                      | 70(26)                             | 42(93)    | 55(47)                        | 41(39)  | 39(35)  |
| C <sub>5</sub> H <sub>10</sub>                 | Cyclopentane                           | 70(44)                             | 42(148)   | 55(43)                        | 41(43)  | 39(31)  |
| C <sub>5</sub> H <sub>10</sub>                 | 2-Methyl-1-butene                      | 70(30)                             | 55(97)    | 42(36)                        | 39(34)  | 41(28)  |
| C <sub>5</sub> H <sub>10</sub>                 | 3-Methyl-1-butene                      | 70(26)                             | 55(102)   | 27(31)                        | 42(28)  | 29(27)  |
| C <sub>5</sub> H <sub>10</sub>                 | 2-Methyl-2-butene                      | 70(31)                             | 55(88)    | 41(31)                        | 39(28)  | 42(27)  |
| C <sub>5</sub> H <sub>10</sub>                 | 1-Pentene                              | 70(27)                             | 42(89)    | 55(53)                        | 41(39)  | 39(31)  |
| C <sub>5</sub> H <sub>10</sub>                 | <i>cis</i> -2-Pentene                  | 70(30)                             | 55(89)    | 42(41)                        | 39(30)  | 29(26)  |
| C <sub>5</sub> H <sub>10</sub>                 | <i>trans</i> -2-Pentene                | 70(31)                             | 55(93)    | 42(41)                        | 39(30)  | 41(28)  |
| C <sub>5</sub> H <sub>10</sub> O               | 3-Methyl-1-butanol                     | 86(3.0)                            | 41(30)    | 43(26)                        | 58(20)  | 29(20)  |

TABLE 7.76 Condensed Table of Mass Spectra (*Continued*)

| Molecular<br>formula                           | Name                            | Mass numbers (and intensities) of: |              |                               |         |         |
|------------------------------------------------|---------------------------------|------------------------------------|--------------|-------------------------------|---------|---------|
|                                                |                                 | Parent<br>peak                     | Base<br>peak | Three next most intense peaks |         |         |
| C <sub>5</sub> H <sub>10</sub> O               | 2-Pentanone                     | 86(16)                             | 43(106)      | 29(23)                        | 27(23)  | 57(20)  |
| C <sub>5</sub> H <sub>10</sub> O               | 3-Pentanone                     | 86(15)                             | 57(87)       | 29(87)                        | 27(32)  | 28(9.4) |
| C <sub>5</sub> H <sub>10</sub> O               | Ethyl-2-propenyl ether          | 86(6.2)                            | 41(52)       | 29(48)                        | 58(44)  | 57(42)  |
| C <sub>5</sub> H <sub>10</sub> O               | Ethyl isopropyl ether           | 86(21)                             | 43(87)       | 44(69)                        | 41(46)  | 27(45)  |
| C <sub>5</sub> H <sub>10</sub> O               | 2-Methyltetrahydrofuran         | 86(8.9)                            | 71(57)       | 43(55)                        | 41(40)  | 27(27)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | Tetrahydrofurfuryl alcohol      | 102(0.02)                          | 71(8.9)      | 43(6.8)                       | 41(4.8) | 27(3.8) |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | 2-Methoxyethyl ethenyl ether    | 102(3.0)                           | 29(69)       | 45(58)                        | 15(48)  | 58(45)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | 2,2-Dimethylpropanoic acid      | 102(2.0)                           | 57(83)       | 41(38)                        | 29(27)  | 39(12)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | 2-Methylbutanoic acid           | 102(0.32)                          | 74(54)       | 57(34)                        | 29(33)  | 41(28)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | <i>n</i> -Butyl formate         | 102(0.27)                          | 56(80)       | 41(48)                        | 31(47)  | 29(42)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | Isobutyl formate                | 102(0.27)                          | 43(58)       | 56(48)                        | 41(46)  | 31(38)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | <i>sec</i> -Butyl formate       | 102(0.17)                          | 45(99)       | 29(49)                        | 27(32)  | 41(31)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | <i>n</i> -Propyl acetate        | 102(0.07)                          | 43(176)      | 61(34)                        | 31(31)  | 27(26)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | Isopropyl acetate               | 102(0.17)                          | 43(155)      | 45(50)                        | 27(22)  | 61(18)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | Ethyl propanoate                | 102(10)                            | 29(151)      | 57(97)                        | 27(52)  | 28(24)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | Methyl 2-methylpropanoate       | 102(8.9)                           | 43(69)       | 71(23)                        | 41(19)  | 59(17)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>  | Methyl butanoate                | 102(1.0)                           | 43(53)       | 74(37)                        | 71(29)  | 27(23)  |
| C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>  | Ethyl carbonate                 | 118(0.30)                          | 29(114)      | 45(80)                        | 31(60)  | 27(46)  |
| C <sub>5</sub> H <sub>10</sub> S               | 2-Methylthiacyclopentane        | 102(37)                            | 87(88)       | 41(30)                        | 45(29)  | 59(18)  |
| C <sub>5</sub> H <sub>10</sub> S               | 3-Methylthiacyclopentane        | 102(40)                            | 60(45)       | 41(31)                        | 45(25)  | 74(23)  |
| C <sub>5</sub> H <sub>10</sub> S               | Thiacyclohexane                 | 102(43)                            | 87(44)       | 68(33)                        | 61(32)  | 41(28)  |
| C <sub>5</sub> H <sub>10</sub> S               | Cyclopentanethiol               | 102(19)                            | 41(48)       | 69(47)                        | 39(26)  | 67(18)  |
| C <sub>5</sub> H <sub>11</sub> N               | Piperidine                      | 85(22)                             | 84(43)       | 57(22)                        | 56(22)  | 44(17)  |
| C <sub>5</sub> H <sub>11</sub> NO              | <i>N</i> -Methylmorpholine      | 101(4.4)                           | 43(18)       | 42(8.6)                       | 15(3.4) | 71(2.9) |
| C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> | 3-Methylbutyl nitrite           | 117(0.0)                           | 29(75)       | 41(68)                        | 57(43)  | 30(42)  |
| C <sub>5</sub> H <sub>12</sub>                 | 2,2-Dimethylpropane             | 72(0.01)                           | 57(126)      | 41(52)                        | 29(49)  | 27(20)  |
| C <sub>5</sub> H <sub>12</sub>                 | 2-Methylbutane                  | 72(4.7)                            | 43(74)       | 42(64)                        | 41(49)  | 57(40)  |
| C <sub>5</sub> H <sub>12</sub>                 | <i>n</i> -Pentane               | 72(10)                             | 43(114)      | 42(66)                        | 41(45)  | 27(39)  |
| C <sub>5</sub> H <sub>12</sub> O               | 2-Methyl-1-butanol              | 88(0.18)                           | 57(57)       | 29(55)                        | 41(53)  | 56(50)  |
| C <sub>5</sub> H <sub>12</sub> O               | 3-Methyl-1-butanol              | 88(0.02)                           | 55(47)       | 42(42)                        | 43(39)  | 41(38)  |
| C <sub>5</sub> H <sub>12</sub> O               | 2-Methyl-2-butanol              | 88(0.0)                            | 59(43)       | 55(37)                        | 45(25)  | 73(22)  |
| C <sub>5</sub> H <sub>12</sub> O               | 1-Pentanol                      | 88(0.0)                            | 42(41)       | 55(30)                        | 41(25)  | 70(23)  |
| C <sub>5</sub> H <sub>12</sub> O               | Methyl <i>n</i> -butyl ether    | 88(3.1)                            | 45(211)      | 56(36)                        | 29(36)  | 27(28)  |
| C <sub>5</sub> H <sub>12</sub> O               | Methyl isobutyl ether           | 88(12)                             | 45(186)      | 41(30)                        | 29(30)  | 15(27)  |
| C <sub>5</sub> H <sub>12</sub> O               | Methyl <i>sec</i> -butyl ether  | 88(2.0)                            | 52(142)      | 29(50)                        | 27(27)  | 41(25)  |
| C <sub>5</sub> H <sub>12</sub> O               | Methyl <i>tert</i> -butyl ether | 88(0.02)                           | 73(119)      | 41(33)                        | 43(32)  | 57(32)  |
| C <sub>5</sub> H <sub>12</sub> O               | Ethyl isopropyl ether           | 88(2.6)                            | 45(143)      | 43(46)                        | 73(40)  | 27(24)  |
| C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>  | Diethoxymethane                 | 104(2.1)                           | 31(104)      | 59(99)                        | 29(62)  | 103(39) |
| C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>  | 1,1-Dimethoxypropane            | 104(0.05)                          | 75(84)       | 73(62)                        | 29(43)  | 45(37)  |
| C <sub>5</sub> H <sub>12</sub> S               | 3,3-Dimethyl-2-thiabutane       | 104(30)                            | 57(83)       | 41(62)                        | 29(42)  | 39(16)  |
| C <sub>5</sub> H <sub>12</sub> S               | 4-Methyl-2-thiapentane          | 104(37)                            | 41(46)       | 56(38)                        | 27(29)  | 39(23)  |
| C <sub>5</sub> H <sub>12</sub> S               | 2-Methyl-3-thiapentane          | 104(82)                            | 89(119)      | 62(79)                        | 43(63)  | 61(58)  |
| C <sub>5</sub> H <sub>12</sub> S               | 2-Thiahexane                    | 104(38)                            | 61(77)       | 56(50)                        | 41(39)  | 27(33)  |
| C <sub>5</sub> H <sub>12</sub> S               | 3-Thiahexane                    | 104(30)                            | 75(72)       | 27(53)                        | 47(50)  | 62(33)  |
| C <sub>5</sub> H <sub>12</sub> S               | 2,2-Dimethyl-1-propanethiol     | 104(31)                            | 57(100)      | 41(55)                        | 55(48)  | 29(42)  |
| C <sub>5</sub> H <sub>12</sub> S               | 2-Methyl-1-butanethiol          | 104(28)                            | 41(65)       | 29(44)                        | 57(40)  | 70(40)  |
| C <sub>5</sub> H <sub>12</sub> S               | 2-Methyl-2-butanethiol          | 104(18)                            | 43(88)       | 71(54)                        | 41(46)  | 55(34)  |
| C <sub>5</sub> H <sub>12</sub> S               | 3-Methyl-2-butanethiol          | 104(23)                            | 61(73)       | 43(55)                        | 27(33)  | 55(28)  |
| C <sub>5</sub> H <sub>12</sub> S               | 1-Pentanethiol                  | 104(35)                            | 42(91)       | 55(44)                        | 41(39)  | 70(39)  |

TABLE 7.76 Condensed Table of Mass Spectra (Continued)

| Molecular formula                             | Name                            | Mass numbers (and intensities) of: |           |                               |         |         |
|-----------------------------------------------|---------------------------------|------------------------------------|-----------|-------------------------------|---------|---------|
|                                               |                                 | Parent peak                        | Base peak | Three next most intense peaks |         |         |
| C <sub>5</sub> H <sub>12</sub> S              | 2-Pentanethiol                  | 104(28)                            | 43(72)    | 61(52)                        | 27(39)  | 55(38)  |
| C <sub>5</sub> H <sub>12</sub> S              | 3-Pentanethiol                  | 104(23)                            | 43(56)    | 41(48)                        | 75(29)  | 47(23)  |
| C <sub>5</sub> H <sub>12</sub> S <sub>2</sub> | 4,4-Dimethyl-2,3-dithiapentane  | 136(12)                            | 57(74)    | 41(38)                        | 29(36)  | 80(13)  |
| C <sub>5</sub> H <sub>12</sub> S <sub>2</sub> | 2-Methyl-3,4-dithiahexane       | 136(20)                            | 94(49)    | 27(46)                        | 43(39)  | 66(37)  |
| C <sub>5</sub> H <sub>14</sub> Pb             | Trimethylethyllead              | 282(0.64)                          | 223(61)   | 253(52)                       | 208(51) | 221(33) |
| C <sub>6</sub> F <sub>6</sub>                 | Hexafluorobenzene               | 186(95)                            | 186(95)   | 117(59)                       | 31(58)  | 93(23)  |
| C <sub>6</sub> F <sub>12</sub>                | Dodecafluorocyclohexane         | 300(0.96)                          | 131(138)  | 69(97)                        | 100(40) | 31(30)  |
| C <sub>6</sub> F <sub>14</sub>                | Tetradecafluoro-2-methylpentane | 338(0.0)                           | 69(317)   | 131(41)                       | 119(36) | 169(29) |
| C <sub>6</sub> F <sub>14</sub>                | Tetradecafluorohexane           | 338(0.13)                          | 69(268)   | 119(74)                       | 169(51) | 131(37) |
| C <sub>6</sub> H <sub>5</sub> Br              | Bromobenzene                    | 156(75)                            | 77(98)    | 158(74)                       | 51(41)  | 50(36)  |
| C <sub>6</sub> H <sub>5</sub> Cl              | Chlorobenzene                   | 112(102)                           | 112(102)  | 77(49)                        | 114(33) | 51(17)  |
| C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> | Nitrobenzene                    | 123(39)                            | 77(93)    | 51(55)                        | 50(23)  | 30(15)  |
| C <sub>6</sub> H <sub>6</sub>                 | Benzene                         | 78(113)                            | 78(113)   | 52(22)                        | 77(20)  | 51(18)  |
| C <sub>6</sub> H <sub>6</sub>                 | 1,5-Hexadiyne                   | 78(58)                             | 39(65)    | 52(38)                        | 51(32)  | 50(26)  |
| C <sub>6</sub> H <sub>6</sub>                 | 2,4-Hexadiyne                   | 78(108)                            | 78(108)   | 51(55)                        | 52(38)  | 50(31)  |
| C <sub>6</sub> H <sub>6</sub> S               | Benzenethiol                    | 110(68)                            | 110(68)   | 66(26)                        | 109(17) | 51(15)  |
| C <sub>6</sub> H <sub>7</sub> N               | Aminobenzene (aniline)          | 93(19)                             | 93(19)    | 66(6.5)                       | 65(3.6) | 39(3.5) |
| C <sub>6</sub> H <sub>7</sub> N               | 2-Methylpyridine                | 93(86)                             | 93(86)    | 66(36)                        | 39(28)  | 51(16)  |
| C <sub>6</sub> H <sub>7</sub> NO              | 1-Methyl-2-pyridone             | 109(71)                            | 109(71)   | 81(49)                        | 39(34)  | 80(29)  |
| C <sub>6</sub> H <sub>8</sub>                 | Methylcyclopentadiene           | 80(53)                             | 79(87)    | 77(29)                        | 39(19)  | 51(11)  |
| C <sub>6</sub> H <sub>8</sub>                 | 1,3-Cyclohexadiene              | 80(53)                             | 79(92)    | 77(35)                        | 39(21)  | 27(18)  |
| C <sub>6</sub> H <sub>8</sub> O               | 2,5-Dimethylfuran               | 96(57)                             | 43(65)    | 95(48)                        | 53(37)  | 81(24)  |
| C <sub>6</sub> H <sub>8</sub> S               | 2,3-Dimethylthiophene           | 112(44)                            | 97(53)    | 111(44)                       | 45(16)  | 27(9.4) |
| C <sub>6</sub> H <sub>8</sub> S               | 2,4-Dimethylthiophene           | 112(27)                            | 111(36)   | 97(18)                        | 45(9.4) | 39(7.0) |
| C <sub>6</sub> H <sub>8</sub> S               | 2,5-Dimethylthiophene           | 112(67)                            | 111(95)   | 97(59)                        | 59(23)  | 45(19)  |
| C <sub>6</sub> H <sub>8</sub> S               | 2-Ethylthiophene                | 112(27)                            | 97(68)    | 45(16)                        | 39(8.9) | 27(5.4) |
| C <sub>6</sub> H <sub>8</sub> S               | 3-Ethylthiophene                | 112(54)                            | 97(147)   | 45(38)                        | 39(20)  | 27(12)  |
| C <sub>6</sub> H <sub>9</sub> N               | 2,5-Dimethylpyrrole             | 95(73)                             | 94(127)   | 26(52)                        | 80(22)  | 42(19)  |
| C <sub>6</sub> H <sub>10</sub>                | Isopropenylcyclopropane         | 82(20)                             | 67(92)    | 41(47)                        | 39(46)  | 27(22)  |
| C <sub>6</sub> H <sub>10</sub>                | 1-Methylcyclopentene            | 82(26)                             | 67(98)    | 39(21)                        | 81(16)  | 41(16)  |
| C <sub>6</sub> H <sub>10</sub>                | Cyclohexene                     | 82(33)                             | 67(83)    | 54(64)                        | 41(31)  | 39(30)  |
| C <sub>6</sub> H <sub>10</sub>                | 2,3-Dimethyl-1,3-butadiene      | 82(41)                             | 67(60)    | 39(55)                        | 41(44)  | 54(22)  |
| C <sub>6</sub> H <sub>10</sub>                | 2-Methyl-1,3-pentadiene         | 82(23)                             | 67(48)    | 39(30)                        | 41(26)  | 27(13)  |
| C <sub>6</sub> H <sub>10</sub>                | 1,5-Hexadiene                   | 82(1.3)                            | 41(98)    | 67(80)                        | 39(60)  | 54(52)  |
| C <sub>6</sub> H <sub>10</sub>                | 3,3-Dimethyl-1-butyne           | 82(0.57)                           | 67(101)   | 41(57)                        | 39(31)  | 27(11)  |
| C <sub>6</sub> H <sub>10</sub>                | 4-Methyl-1-pentyne              | 82(2.3)                            | 67(82)    | 41(74)                        | 43(64)  | 39(55)  |
| C <sub>6</sub> H <sub>10</sub>                | 1-Hexyne                        | 82(1.0)                            | 67(131)   | 41(88)                        | 27(85)  | 43(67)  |
| C <sub>6</sub> H <sub>10</sub>                | 2-Hexyne                        | 82(56)                             | 67(58)    | 53(50)                        | 27(39)  | 41(36)  |
| C <sub>6</sub> H <sub>10</sub>                | 3-Hexyne                        | 82(55)                             | 67(59)    | 41(55)                        | 39(37)  | 53(20)  |
| C <sub>6</sub> H <sub>10</sub> O              | Cyclohexanone                   | 98(32)                             | 55(102)   | 42(86)                        | 41(35)  | 27(34)  |
| C <sub>6</sub> H <sub>10</sub> O              | 4-Methyl-3-penten-2-one         | 98(40)                             | 55(82)    | 83(82)                        | 43(64)  | 29(38)  |
| C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> | 2,5-Hexanedione                 | 114(4.0)                           | 43(148)   | 15(25)                        | 99(22)  | 14(14)  |
| C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> | Propanoic anhydride             | 130(0.0)                           | 57(190)   | 29(119)                       | 27(62)  | 28(26)  |
| C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> | Ethyl acetoacetate              | 130(8.3)                           | 43(150)   | 29(52)                        | 27(32)  | 15(27)  |
| C <sub>6</sub> H <sub>11</sub> N              | 4-Methylpentanenitrile          | 97(0.13)                           | 55(98)    | 41(51)                        | 43(45)  | 27(39)  |
| C <sub>6</sub> H <sub>11</sub> N              | Hexanenitrile                   | 97(0.54)                           | 41(73)    | 54(49)                        | 27(43)  | 55(40)  |
| C <sub>6</sub> H <sub>12</sub>                | 1,1,2-Trimethylcyclopropane     | 84(38)                             | 41(132)   | 69(81)                        | 39(34)  | 27(24)  |
| C <sub>6</sub> H <sub>12</sub>                | 1-Methyl-1-ethylcyclopropane    | 84(25)                             | 41(78)    | 55(58)                        | 69(53)  | 27(33)  |
| C <sub>6</sub> H <sub>12</sub>                | Isopropylcyclopropane           | 84(2.0)                            | 56(114)   | 41(84)                        | 39(30)  | 43(28)  |

TABLE 7.76 Condensed Table of Mass Spectra (*Continued*)

| Molecular formula                             | Name                                       | Mass numbers (and intensities) of: |           |                               |          |         |
|-----------------------------------------------|--------------------------------------------|------------------------------------|-----------|-------------------------------|----------|---------|
|                                               |                                            | Parent peak                        | Base peak | Three next most intense peaks |          |         |
| C <sub>6</sub> H <sub>12</sub>                | Ethylcyclobutane                           | 84(3.8)                            | 56(138)   | 41(89)                        | 27(35)   | 55(34)  |
| C <sub>6</sub> H <sub>12</sub>                | Methylcyclopentane                         | 84(18)                             | 56(116)   | 41(74)                        | 69(37)   | 42(33)  |
| C <sub>6</sub> H <sub>12</sub>                | Cyclohexane                                | 84(58)                             | 56(75)    | 41(44)                        | 55(25)   | 42(21)  |
| C <sub>6</sub> H <sub>12</sub>                | 2,3-Dimethyl-1-butene                      | 84(27)                             | 41(117)   | 69(96)                        | 39(36)   | 27(24)  |
| C <sub>6</sub> H <sub>12</sub>                | 3,3-Dimethyl-1-butene                      | 84(23)                             | 41(112)   | 69(107)                       | 39(28)   | 27(26)  |
| C <sub>6</sub> H <sub>12</sub>                | 2-Ethyl-1-butene                           | 84(30)                             | 41(74)    | 69(66)                        | 55(56)   | 27(38)  |
| C <sub>6</sub> H <sub>12</sub>                | 2,3-Dimethyl-2-butene                      | 84(32)                             | 41(108)   | 69(88)                        | 39(35)   | 27(20)  |
| C <sub>6</sub> H <sub>12</sub>                | 2-Methyl-1-pentene                         | 84(29)                             | 56(91)    | 41(73)                        | 55(39)   | 39(36)  |
| C <sub>6</sub> H <sub>12</sub>                | 3-Methyl-1-pentene                         | 84(25)                             | 55(85)    | 41(67)                        | 69(60)   | 27(43)  |
| C <sub>6</sub> H <sub>12</sub>                | 4-Methyl-1-pentene                         | 84(12)                             | 43(110)   | 41(80)                        | 56(47)   | 27(37)  |
| C <sub>6</sub> H <sub>12</sub>                | 2-Methyl-2-pentene                         | 84(36)                             | 41(120)   | 69(111)                       | 39(35)   | 27(28)  |
| C <sub>6</sub> H <sub>12</sub>                | 3-Methyl- <i>cis</i> -2-pentene            | 84(37)                             | 41(104)   | 69(82)                        | 55(46)   | 27(36)  |
| C <sub>6</sub> H <sub>12</sub>                | 3-Methyl- <i>trans</i> -2-pentene          | 84(38)                             | 41(102)   | 69(81)                        | 55(47)   | 27(35)  |
| C <sub>6</sub> H <sub>12</sub>                | 4-Methyl- <i>cis</i> -2-pentene            | 84(35)                             | 41(122)   | 69(114)                       | 39(35)   | 27(26)  |
| C <sub>6</sub> H <sub>12</sub>                | 4-Methyl- <i>trans</i> -2-pentene          | 84(34)                             | 41(123)   | 69(112)                       | 39(34)   | 27(26)  |
| C <sub>6</sub> H <sub>12</sub>                | 1-Hexene                                   | 84(20)                             | 41(70)    | 56(60)                        | 42(52)   | 27(48)  |
| C <sub>6</sub> H <sub>12</sub>                | <i>cis</i> -2-Hexene                       | 84(27)                             | 55(91)    | 42(51)                        | 41(45)   | 27(45)  |
| C <sub>6</sub> H <sub>12</sub>                | <i>trans</i> -2-Hexene                     | 84(32)                             | 55(112)   | 42(54)                        | 41(46)   | 27(41)  |
| C <sub>6</sub> H <sub>12</sub>                | <i>cis</i> -3-Hexene                       | 84(28)                             | 55(81)    | 41(62)                        | 42(54)   | 27(32)  |
| C <sub>6</sub> H <sub>12</sub>                | <i>trans</i> -3-Hexene                     | 84(32)                             | 55(89)    | 41(72)                        | 42(62)   | 27(35)  |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> | Acetone azine (ketazine)                   | 112(31)                            | 56(99)    | 15(31)                        | 97(31)   | 39(26)  |
| C <sub>6</sub> H <sub>12</sub> O              | Cyclopentylmethanol                        | 100(0.02)                          | 41(35)    | 68(32)                        | 69(31)   | 67(24)  |
| C <sub>6</sub> H <sub>12</sub> O              | 4-Methyl-2-pentanone                       | 100(12)                            | 43(115)   | 58(37)                        | 41(22)   | 57(22)  |
| C <sub>6</sub> H <sub>12</sub> O              | Ethenyl <i>n</i> -butyl ether              | 100(5.7)                           | 29(80)    | 41(59)                        | 56(45)   | 57(35)  |
| C <sub>6</sub> H <sub>12</sub> O              | Ethenyl isobutyl ether                     | 100(5.8)                           | 29(73)    | 41(65)                        | 57(58)   | 56(40)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> | 4-Hydroxy-4-methyl-2-pentanone             | 116(0.0)                           | 43(149)   | 15(45)                        | 58(32)   | 27(14)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> | <i>n</i> -Butyl acetate                    | 116(0.03)                          | 43(172)   | 56(58)                        | 41(30)   | 27(27)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> | <i>n</i> -Propyl propanoate                | 116(0.03)                          | 57(147)   | 29(84)                        | 27(57)   | 75(47)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> | Isopropyl propanoate                       | 116(0.26)                          | 57(116)   | 43(88)                        | 29(54)   | 27(46)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> | Methyl 2,2-dimethylpropanoate              | 116(3.2)                           | 57(85)    | 41(32)                        | 29(24)   | 56(21)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> | Ethyl butanoate                            | 116(2.2)                           | 43(50)    | 71(45)                        | 29(43)   | 27(31)  |
| C <sub>6</sub> H <sub>12</sub> O <sub>3</sub> | 2,4,6-Trimethyl-1,3,5-trioxacyclohexane    | 132(0.12)                          | 45(196)   | 43(107)                       | 29(35)   | 89(23)  |
| C <sub>6</sub> H <sub>12</sub> S              | 1-Cyclopentyl-1-thiaethane                 | 116(31)                            | 68(72)    | 41(64)                        | 39(37)   | 67(37)  |
| C <sub>6</sub> H <sub>12</sub> S              | <i>cis</i> -2,5-Dimethylthiacyclopentane   | 116(32)                            | 101(85)   | 59(34)                        | 41(26)   | 74(24)  |
| C <sub>6</sub> H <sub>12</sub> S              | <i>trans</i> -2,5-Dimethylthiacyclopentane | 116(32)                            | 101(85)   | 59(34)                        | 74(25)   | 41(25)  |
| C <sub>6</sub> H <sub>12</sub> S              | 2-Methylthiacyclohexane                    | 116(42)                            | 101(81)   | 41(37)                        | 27(32)   | 67(30)  |
| C <sub>6</sub> H <sub>12</sub> S              | 3-Methylthiacyclohexane                    | 116(41)                            | 101(55)   | 41(47)                        | 39(33)   | 45(28)  |
| C <sub>6</sub> H <sub>12</sub> S              | 4-Methylthiacyclohexane                    | 116(46)                            | 116(46)   | 101(44)                       | 41(40)   | 27(39)  |
| C <sub>6</sub> H <sub>12</sub> S              | Thiacycloheptane                           | 116(60)                            | 87(75)    | 41(66)                        | 67(48)   | 47(46)  |
| C <sub>6</sub> H <sub>12</sub> S              | 1-Methylcyclopentanethiol                  | 116(20)                            | 83(76)    | 55(58)                        | 41(39)   | 67(33)  |
| C <sub>6</sub> H <sub>12</sub> S              | <i>cis</i> -2-Methylcyclopentanethiol      | 116(32)                            | 55(55)    | 83(54)                        | 60(48)   | 41(47)  |
| C <sub>6</sub> H <sub>12</sub> S              | <i>trans</i> -2-Methylcyclopentanethiol    | 116(28)                            | 67(48)    | 55(46)                        | 41(42)   | 83(40)  |
| C <sub>6</sub> H <sub>12</sub> S              | Cyclohexanethiol                           | 116(21)                            | 55(56)    | 41(45)                        | 67(35)   | 83(32)  |
| C <sub>6</sub> H <sub>13</sub> N              | Cyclohexylamine                            | 99(8.9)                            | 56(92)    | 43(25)                        | 28(13)   | 30(13)  |
| C <sub>6</sub> H <sub>13</sub> N              | 3-Methylpiperidine                         | 99(23)                             | 44(49)    | 30(34)                        | 28(27)   | 57(26)  |
| C <sub>6</sub> H <sub>13</sub> NO             | <i>N</i> -Ethylmorpholine                  | 115(2.0)                           | 42(9.8)   | 57(7.0)                       | 100(5.2) | 28(4.3) |
| C <sub>6</sub> H <sub>14</sub>                | 2,2-Dimethylbutane                         | 86(0.04)                           | 43(85)    | 57(82)                        | 71(61)   | 41(51)  |
| C <sub>6</sub> H <sub>14</sub>                | 2,3-Dimethylbutane                         | 86(5.3)                            | 43(157)   | 42(136)                       | 41(49)   | 27(40)  |

TABLE 7.76 Condensed Table of Mass Spectra (Continued)

| Molecular formula                             | Name                               | Mass numbers (and intensities) of: |           |                               |         |         |
|-----------------------------------------------|------------------------------------|------------------------------------|-----------|-------------------------------|---------|---------|
|                                               |                                    | Parent peak                        | Base peak | Three next most intense peaks |         |         |
| C <sub>6</sub> H <sub>14</sub>                | 2-Methylpentane                    | 86(4.4)                            | 43(147)   | 42(78)                        | 41(47)  | 27(40)  |
| C <sub>6</sub> H <sub>14</sub>                | 3-Methylpentane                    | 86(3.2)                            | 57(105)   | 56(80)                        | 41(67)  | 29(64)  |
| C <sub>6</sub> H <sub>14</sub>                | <i>n</i> -Hexane                   | 86(12)                             | 57(87)    | 43(71)                        | 41(64)  | 29(55)  |
| C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> | <i>cis</i> -2,5-Dimethylpiperazine | 114(0.38)                          | 58(10)    | 28(7.7)                       | 30(4.7) | 44(4.2) |
| C <sub>6</sub> H <sub>14</sub> O              | 2-Ethyl-1-butanol                  | 102(0.0)                           | 43(114)   | 70(40)                        | 29(39)  | 27(38)  |
| C <sub>6</sub> H <sub>14</sub> O              | 2-Methyl-1-pentanol                | 102(0.0)                           | 42(110)   | 41(40)                        | 29(34)  | 27(33)  |
| C <sub>6</sub> H <sub>14</sub> O              | 3-Methyl-1-pentanol                | 102(0.0)                           | 56(26)    | 41(20)                        | 29(19)  | 55(18)  |
| C <sub>6</sub> H <sub>14</sub> O              | 4-Methyl-2-pentanol                | 102(0.08)                          | 45(111)   | 43(34)                        | 41(17)  | 27(14)  |
| C <sub>6</sub> H <sub>14</sub> O              | 1-Hexanol                          | 102(0.0)                           | 56(63)    | 43(52)                        | 41(37)  | 55(36)  |
| C <sub>6</sub> H <sub>14</sub> O              | Ethyl <i>n</i> -butyl ether        | 102(3.8)                           | 59(108)   | 31(87)                        | 29(61)  | 27(42)  |
| C <sub>6</sub> H <sub>14</sub> O              | Ethyl <i>sec</i> -butyl ether      | 102(1.5)                           | 45(150)   | 73(76)                        | 29(51)  | 27(39)  |
| C <sub>6</sub> H <sub>14</sub> O              | Ethyl isobutyl ether               | 102(8.7)                           | 59(124)   | 31(95)                        | 29(53)  | 27(38)  |
| C <sub>6</sub> H <sub>14</sub> O              | Diisopropyl ether                  | 102(1.4)                           | 45(125)   | 43(66)                        | 87(23)  | 27(19)  |
| C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> | 1,1-Diethoxyethane                 | 118(0.0)                           | 45(132)   | 73(69)                        | 29(36)  | 27(27)  |
| C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> | 1,2-Diethoxyethane                 | 118(1.2)                           | 31(124)   | 59(88)                        | 29(72)  | 45(53)  |
| C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> | <i>bis</i> -(2-Methoxyethyl) ether | 134(0.0)                           | 59(140)   | 29(74)                        | 58(57)  | 15(56)  |
| C <sub>6</sub> H <sub>14</sub> S              | 2,2-Dimethyl-3-thiapentane         | 118(33)                            | 57(147)   | 41(70)                        | 29(54)  | 27(40)  |
| C <sub>6</sub> H <sub>14</sub> S              | 2,4-Dimethyl-3-thiapentne          | 118(33)                            | 43(94)    | 61(85)                        | 41(48)  | 103(44) |
| C <sub>6</sub> H <sub>14</sub> S              | 2-Methyl-3-thiahexane              | 118(206)                           | 43(540)   | 41(317)                       | 42(301) | 27(287) |
| C <sub>6</sub> H <sub>14</sub> S              | 4-Methyl-3-thiahexane              | 118(195)                           | 89(585)   | 29(343)                       | 27(296) | 41(279) |
| C <sub>6</sub> H <sub>14</sub> S              | 5-Methyl-3-thiahexane              | 118(171)                           | 75(520)   | 41(230)                       | 47(224) | 56(217) |
| C <sub>6</sub> H <sub>14</sub> S              | 3-Thiaheptane                      | 118(35)                            | 75(55)    | 29(33)                        | 27(33)  | 62(28)  |
| C <sub>6</sub> H <sub>14</sub> S              | 4-Thiaheptane                      | 118(47)                            | 43(86)    | 89(74)                        | 41(57)  | 27(55)  |
| C <sub>6</sub> H <sub>14</sub> S              | 2-Methyl-1-pentanethiol            | 118(19)                            | 43(96)    | 41(51)                        | 56(32)  | 27(31)  |
| C <sub>6</sub> H <sub>14</sub> S              | 4-Methyl-1-pentanethiol            | 118(30)                            | 56(142)   | 41(57)                        | 43(57)  | 27(32)  |
| C <sub>6</sub> H <sub>14</sub> S              | 4-Methyl-2-pentanethiol            | 118(6.3)                           | 43(68)    | 69(61)                        | 41(56)  | 84(42)  |
| C <sub>6</sub> H <sub>14</sub> S              | 2-Methyl-3-pentanethiol            | 118(20)                            | 41(64)    | 43(63)                        | 75(50)  | 27(28)  |
| C <sub>6</sub> H <sub>14</sub> S              | 1-Hexanethiol                      | 118(16)                            | 56(66)    | 41(41)                        | 27(40)  | 43(38)  |
| C <sub>6</sub> H <sub>14</sub> S <sub>2</sub> | 2,5-Dimethyl-3,4-dithiahexane      | 150(31)                            | 43(152)   | 108(41)                       | 41(36)  | 27(30)  |
| C <sub>6</sub> H <sub>14</sub> S <sub>2</sub> | 5-Methyl-3,4-dithiaheptane         | 150(14)                            | 29(86)    | 94(66)                        | 66(57)  | 27(41)  |
| C <sub>6</sub> H <sub>14</sub> S <sub>2</sub> | 6-Methyl-3,4-dithiaheptane         | 150(4.9)                           | 29(42)    | 66(40)                        | 122(30) | 94(29)  |
| C <sub>6</sub> H <sub>14</sub> S <sub>2</sub> | 4,5-Dithiaoctane                   | 150(44)                            | 43(167)   | 27(65)                        | 41(64)  | 108(35) |
| C <sub>6</sub> H <sub>15</sub> N              | Triethylamine                      | 101(21)                            | 86(134)   | 30(46)                        | 27(36)  | 58(35)  |
| C <sub>6</sub> H <sub>15</sub> N              | Di- <i>n</i> -propylamine          | 101(7.1)                           | 30(89)    | 72(70)                        | 44(36)  | 43(28)  |
| C <sub>6</sub> H <sub>15</sub> N              | Diisopropylamine                   | 101(5.0)                           | 44(171)   | 86(52)                        | 58(24)  | 42(22)  |
| C <sub>6</sub> H <sub>16</sub> Pb             | Dimethyl-diethyllead               | 296(0.98)                          | 267(89)   | 223(83)                       | 208(79) | 221(44) |
| C <sub>7</sub> F <sub>14</sub>                | Tetradecafluoromethylcyclohexane   | 350(0.0)                           | 69(244)   | 131(107)                      | 181(48) | 100(38) |
| C <sub>7</sub> F <sub>16</sub>                | Hexadecafluoroheptane              | 388(0.0)                           | 69(330)   | 119(89)                       | 169(68) | 131(44) |
| C <sub>7</sub> H <sub>5</sub> N               | Benzonitrile                       | 103(246)                           | 103(246)  | 76(80)                        | 50(42)  | 51(24)  |
| C <sub>7</sub> H <sub>7</sub> Br              | 1-Methyl-2-bromobenzene            | 170(48)                            | 91(97)    | 172(46)                       | 39(21)  | 63(20)  |
| C <sub>7</sub> H <sub>7</sub> Br              | 1-Methyl-4-bromobenzene            | 170(46)                            | 91(97)    | 172(45)                       | 39(20)  | 65(19)  |
| C <sub>7</sub> H <sub>7</sub> Cl              | 1-Methyl-2-chlorobenzene           | 126(44)                            | 91(121)   | 63(20)                        | 39(19)  | 89(18)  |
| C <sub>7</sub> H <sub>7</sub> Cl              | 1-Methyl-3-chlorobenzene           | 126(51)                            | 91(120)   | 63(19)                        | 39(18)  | 128(16) |
| C <sub>7</sub> H <sub>7</sub> Cl              | 1-Methyl-4-chlorobenzene           | 126(44)                            | 91(120)   | 125(19)                       | 63(18)  | 39(17)  |
| C <sub>7</sub> H <sub>7</sub> F               | 1-Methyl-3-fluorobenzene           | 110(79)                            | 109(129)  | 83(17)                        | 57(12)  | 39(12)  |
| C <sub>7</sub> H <sub>7</sub> F               | 1-Methyl-4-fluorobenzene           | 110(73)                            | 109(122)  | 83(16)                        | 57(12)  | 39(9.3) |
| C <sub>7</sub> H <sub>8</sub>                 | Methylbenzene (toluene)            | 92(82)                             | 91(108)   | 39(20)                        | 65(14)  | 51(10)  |
| C <sub>7</sub> H <sub>8</sub> S               | 1-Phenyl-1-thiaethane              | 124(76)                            | 124(76)   | 109(34)                       | 78(25)  | 91(19)  |
| C <sub>7</sub> H <sub>9</sub> N               | 2,4-Dimethylpyridine               | 107(76)                            | 107(76)   | 106(29)                       | 79(16)  | 92(13)  |



TABLE 7.76 Condensed Table of Mass Spectra (*Continued*)

| Molecular formula                | Name                                   | Mass numbers (and intensities) of: |           |                               |        |        |
|----------------------------------|----------------------------------------|------------------------------------|-----------|-------------------------------|--------|--------|
|                                  |                                        | Parent peak                        | Base peak | Three next most intense peaks |        |        |
| C <sub>7</sub> H <sub>10</sub> S | 2,3,4-Trimethylthiophene               | 126(50)                            | 111(81)   | 125(47)                       | 45(22) | 39(18) |
| C <sub>7</sub> H <sub>12</sub>   | Ethenylcyclopentane                    | 96(13)                             | 67(118)   | 39(44)                        | 68(38) | 54(35) |
| C <sub>7</sub> H <sub>12</sub>   | Ethylidenecyclopentane                 | 96(40)                             | 67(180)   | 39(44)                        | 41(30) | 27(30) |
| C <sub>7</sub> H <sub>12</sub>   | Bicyclo[2.2.1]heptane                  | 96(12)                             | 67(64)    | 68(50)                        | 81(44) | 54(30) |
| C <sub>7</sub> H <sub>12</sub>   | 3-Ethylcyclopentene                    | 96(29)                             | 67(193)   | 39(36)                        | 41(35) | 27(26) |
| C <sub>7</sub> H <sub>12</sub>   | 1-Methylcyclohexene                    | 96(32)                             | 81(83)    | 68(38)                        | 67(37) | 39(33) |
| C <sub>7</sub> H <sub>12</sub>   | 4-Methylcyclohexene                    | 96(28)                             | 81(84)    | 54(50)                        | 39(44) | 55(34) |
| C <sub>7</sub> H <sub>12</sub>   | 4-Methyl-2-hexyne                      | 96(13)                             | 81(71)    | 67(52)                        | 41(48) | 39(35) |
| C <sub>7</sub> H <sub>12</sub>   | 5-Methyl-2-hexyne                      | 96(42)                             | 43(49)    | 81(43)                        | 27(39) | 39(38) |
| C <sub>7</sub> H <sub>12</sub>   | 1-Heptyne                              | 96(0.44)                           | 41(75)    | 81(70)                        | 29(65) | 27(47) |
| C <sub>7</sub> H <sub>14</sub>   | 1,1,2,2,-Tetramethylcyclopropane       | 98(21)                             | 55(92)    | 83(90)                        | 41(69) | 39(41) |
| C <sub>7</sub> H <sub>14</sub>   | <i>cis</i> -1,2-Dimethylcyclopentane   | 98(19)                             | 56(85)    | 70(77)                        | 41(65) | 55(65) |
| C <sub>7</sub> H <sub>14</sub>   | <i>trans</i> -1,2-Dimethylcyclopentane | 98(25)                             | 56(93)    | 41(63)                        | 55(61) | 70(54) |
| C <sub>7</sub> H <sub>14</sub>   | <i>cis</i> -1,3-Dimethylcyclopentane   | 98(12)                             | 56(81)    | 70(78)                        | 41(64) | 55(59) |
| C <sub>7</sub> H <sub>14</sub>   | <i>trans</i> -1,3-Dimethylcyclopentane | 98(13)                             | 56(81)    | 70(68)                        | 41(63) | 55(58) |
| C <sub>7</sub> H <sub>14</sub>   | 1,1-Dimethylcyclopentane               | 98(6.7)                            | 56(81)    | 55(63)                        | 69(56) | 41(55) |
| C <sub>7</sub> H <sub>14</sub>   | Ethylcyclopentane                      | 98(14)                             | 69(83)    | 41(78)                        | 68(60) | 55(46) |
| C <sub>7</sub> H <sub>14</sub>   | Methylcyclohexane                      | 98(41)                             | 83(94)    | 55(78)                        | 41(55) | 42(34) |
| C <sub>7</sub> H <sub>14</sub>   | Cycloheptane                           | 98(37)                             | 41(57)    | 55(54)                        | 56(50) | 42(49) |
| C <sub>7</sub> H <sub>14</sub>   | 2,3,3-Trimethyl-1-butene               | 98(20)                             | 83(101)   | 55(83)                        | 41(61) | 39(33) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Methyl-2-ethyl-1-butene              | 98(22)                             | 41(71)    | 69(71)                        | 55(62) | 27(38) |
| C <sub>7</sub> H <sub>14</sub>   | 2,3-Dimethyl-1-pentene                 | 98(13)                             | 41(92)    | 69(86)                        | 55(40) | 39(35) |
| C <sub>7</sub> H <sub>14</sub>   | 2,4-Dimethyl-1-pentene                 | 98(9.1)                            | 56(117)   | 43(68)                        | 41(61) | 39(39) |
| C <sub>7</sub> H <sub>14</sub>   | 3,3-Dimethyl-1-pentene                 | 98(9.4)                            | 69(104)   | 41(85)                        | 55(42) | 27(36) |
| C <sub>7</sub> H <sub>14</sub>   | 3,4-Dimethyl-1-pentene                 | 98(0.61)                           | 56(75)    | 55(62)                        | 43(55) | 41(54) |
| C <sub>7</sub> H <sub>14</sub>   | 4,4-Dimethyl-1-pentene                 | 98(2.6)                            | 57(161)   | 41(86)                        | 29(52) | 55(49) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Ethyl-1-pentene                      | 98(19)                             | 41(116)   | 69(91)                        | 27(43) | 39(37) |
| C <sub>7</sub> H <sub>14</sub>   | 2,3-Dimethyl-2-pentene                 | 98(31)                             | 83(80)    | 55(75)                        | 41(63) | 39(34) |
| C <sub>7</sub> H <sub>14</sub>   | 2,4-Dimethyl-2-pentene                 | 98(26)                             | 83(97)    | 55(71)                        | 41(52) | 39(34) |
| C <sub>7</sub> H <sub>14</sub>   | 3,4-Dimethyl- <i>cis</i> -2-pentene    | 98(30)                             | 83(87)    | 55(82)                        | 41(52) | 27(32) |
| C <sub>7</sub> H <sub>14</sub>   | 3,4-Dimethyl- <i>trans</i> -2-pentene  | 98(31)                             | 83(89)    | 55(83)                        | 41(52) | 27(34) |
| C <sub>7</sub> H <sub>14</sub>   | 4,4-Dimethyl- <i>cis</i> -2-pentene    | 98(27)                             | 83(96)    | 55(92)                        | 41(62) | 39(35) |
| C <sub>7</sub> H <sub>14</sub>   | 4,4-Dimethyl- <i>trans</i> -2-pentene  | 98(28)                             | 83(105)   | 55(89)                        | 41(58) | 39(31) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Ethyl-2-pentene                      | 98(33)                             | 41(86)    | 69(80)                        | 55(74) | 27(33) |
| C <sub>7</sub> H <sub>14</sub>   | 2-Methyl-1-hexene                      | 98(4.6)                            | 56(105)   | 41(54)                        | 27(30) | 39(27) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Methyl-1-hexene                      | 98(7.7)                            | 55(76)    | 41(60)                        | 69(57) | 56(48) |
| C <sub>7</sub> H <sub>14</sub>   | 4-Methyl-1-hexene                      | 98(4.9)                            | 41(98)    | 57(94)                        | 56(80) | 29(70) |
| C <sub>7</sub> H <sub>14</sub>   | 5-Methyl-1-hexene                      | 98(1.6)                            | 56(91)    | 41(75)                        | 55(47) | 27(42) |
| C <sub>7</sub> H <sub>14</sub>   | 2-Methyl-2-hexene                      | 98(28)                             | 69(113)   | 41(99)                        | 27(36) | 39(33) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Methyl- <i>cis</i> -2-hexene         | 98(30)                             | 41(95)    | 69(90)                        | 55(42) | 27(36) |
| C <sub>7</sub> H <sub>14</sub>   | 4-Methyl- <i>trans</i> -2-hexene       | 98(23)                             | 69(118)   | 41(106)                       | 55(40) | 39(35) |
| C <sub>7</sub> H <sub>14</sub>   | 5-Methyl-2-hexene                      | 98(13)                             | 56(90)    | 55(74)                        | 43(71) | 41(57) |
| C <sub>7</sub> H <sub>14</sub>   | 2-Methyl- <i>trans</i> -3-hexene       | 98(24)                             | 69(86)    | 41(74)                        | 55(62) | 56(37) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Methyl- <i>cis</i> -3-hexene         | 98(28)                             | 69(98)    | 41(82)                        | 39(33) | 27(33) |
| C <sub>7</sub> H <sub>14</sub>   | 3-Methyl- <i>trans</i> -3-hexene       | 98(28)                             | 69(97)    | 41(86)                        | 55(63) | 39(35) |
| C <sub>7</sub> H <sub>14</sub>   | 1-Heptene                              | 98(15)                             | 41(91)    | 56(79)                        | 29(64) | 55(54) |
| C <sub>7</sub> H <sub>14</sub>   | <i>trans</i> -2-Heptene                | 98(27)                             | 55(64)    | 56(59)                        | 41(50) | 27(35) |
| C <sub>7</sub> H <sub>14</sub>   | <i>trans</i> -3-Heptene                | 98(27)                             | 41(98)    | 56(65)                        | 69(55) | 55(47) |
| C <sub>7</sub> H <sub>14</sub> O | 2,4-Dimethyl-3-pentanone               | 114(13)                            | 43(226)   | 71(62)                        | 27(49) | 41(42) |



**TABLE 7.76** Condensed Table of Mass Spectra (*Continued*)

| Molecular formula                             | Name                                   | Mass numbers (and intensities) of: |           |                               |          |          |
|-----------------------------------------------|----------------------------------------|------------------------------------|-----------|-------------------------------|----------|----------|
|                                               |                                        | Parent peak                        | Base peak | Three next most intense peaks |          |          |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> | <i>n</i> -Butyl propanoate             | 130(0.03)                          | 57(152)   | 29(98)                        | 56(54)   | 27(52)   |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> | Isobutyl propanoate                    | 130(0.07)                          | 57(187)   | 29(87)                        | 56(27)   | 27(47)   |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> | <i>n</i> -Propyl <i>n</i> -butanoate   | 130(0.05)                          | 43(96)    | 71(90)                        | 27(54)   | 89(48)   |
| C <sub>7</sub> H <sub>14</sub> O <sub>3</sub> | <i>n</i> -Propyl carbonate             | 146(0.02)                          | 43(171)   | 27(61)                        | 63(55)   | 41(49)   |
| C <sub>7</sub> H <sub>14</sub> S              | <i>cis</i> -2-Methylcyclohexanethiol   | 130(28)                            | 55(138)   | 97(70)                        | 81(44)   | 41(44)   |
| C <sub>7</sub> H <sub>15</sub> N              | 2,6-Dimethylpiperidine                 | 113(5.3)                           | 98(73)    | 44(43)                        | 42(34)   | 28(26)   |
| C <sub>7</sub> H <sub>16</sub>                | 2,2,3-Trimethylbutane                  | 100(0.03)                          | 57(110)   | 43(84)                        | 56(67)   | 41(64)   |
| C <sub>7</sub> H <sub>16</sub>                | 2,2-Dimethylpentane                    | 100(0.06)                          | 57(130)   | 43(95)                        | 41(59)   | 56(52)   |
| C <sub>7</sub> H <sub>16</sub>                | 2,3-Dimethylpentane                    | 100(2.1)                           | 43(94)    | 56(93)                        | 57(67)   | 41(64)   |
| C <sub>7</sub> H <sub>16</sub>                | 2,4-Dimethylpentane                    | 100(1.6)                           | 43(139)   | 57(93)                        | 41(59)   | 56(50)   |
| C <sub>7</sub> H <sub>16</sub>                | 3,3-Dimethylpentane                    | 100(0.03)                          | 43(166)   | 71(103)                       | 27(38)   | 41(36)   |
| C <sub>7</sub> H <sub>16</sub>                | 3-Ethylpentane                         | 100(3.1)                           | 43(175)   | 70(77)                        | 70(77)   | 29(45)   |
| C <sub>7</sub> H <sub>16</sub>                | 2-Methylhexane                         | 100(5.9)                           | 43(154)   | 42(59)                        | 41(57)   | 85(49)   |
| C <sub>7</sub> H <sub>16</sub>                | 3-Methylhexane                         | 100(4.0)                           | 43(110)   | 57(52)                        | 71(52)   | 41(50)   |
| C <sub>7</sub> H <sub>16</sub>                | <i>n</i> -Heptane                      | 100(17)                            | 43(126)   | 41(65)                        | 57(60)   | 29(58)   |
| C <sub>7</sub> H <sub>16</sub> O              | 2-Heptanol                             | 116(0.01)                          | 45(131)   | 43(29)                        | 27(25)   | 29(23)   |
| C <sub>7</sub> H <sub>16</sub> O              | 3-Heptanol                             | 116(0.01)                          | 59(61)    | 69(41)                        | 41(29)   | 31(25)   |
| C <sub>7</sub> H <sub>16</sub> O              | 4-Heptanol                             | 116(0.02)                          | 55(102)   | 73(72)                        | 43(45)   | 27(32)   |
| C <sub>7</sub> H <sub>16</sub> O              | <i>n</i> -Propyl <i>n</i> -butyl ether | 116(3.7)                           | 43(120)   | 57(102)                       | 41(51)   | 29(49)   |
| C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> | Di- <i>n</i> -propoxymethane           | 132(0.58)                          | 43(194)   | 73(114)                       | 27(45)   | 41(34)   |
| C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> | Diisopropoxymethane                    | 132(0.16)                          | 43(133)   | 45(84)                        | 73(71)   | 27(28)   |
| C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> | 1,1-Diethoxypropane                    | 132(0.0)                           | 59(138)   | 47(88)                        | 87(84)   | 29(74)   |
| C <sub>7</sub> H <sub>16</sub> S              | 2,2,4-Trimethyl-3-thiapentane          | 132(30)                            | 57(149)   | 41(74)                        | 29(35)   | 43(32)   |
| C <sub>7</sub> H <sub>16</sub> S              | 2,4-Dimethyl-3-thiahexane              | 132(30)                            | 61(94)    | 103(60)                       | 41(51)   | 43(46)   |
| C <sub>7</sub> H <sub>16</sub> S              | 2-Thiaoctane                           | 132(34)                            | 61(73)    | 56(53)                        | 27(46)   | 41(44)   |
| C <sub>7</sub> H <sub>16</sub> S              | 1-Heptanethiol                         | 132(14)                            | 41(48)    | 27(40)                        | 56(39)   | 70(38)   |
| C <sub>7</sub> H <sub>18</sub> Pb             | Methyltriethyllead                     | 310(0.84)                          | 281(86)   | 208(76)                       | 223(66)  | 237(60)  |
| C <sub>7</sub> H <sub>18</sub> Pb             | <i>n</i> -Butyltrimethyllead           | 310(0.14)                          | 253(76)   | 223(75)                       | 208(68)  | 295(52)  |
| C <sub>7</sub> H <sub>18</sub> Pb             | <i>sec</i> -Butyltrimethyllead         | 310(1.8)                           | 253(94)   | 223(85)                       | 208(74)  | 251(45)  |
| C <sub>7</sub> H <sub>18</sub> Pb             | <i>tert</i> -Butyltrimethyllead        | 310(0.09)                          | 252(95)   | 223(82)                       | 208(65)  | 250(46)  |
| C <sub>8</sub> H <sub>10</sub>                | 1,2-Dimethylbenzene                    | 106(52)                            | 91(91)    | 105(22)                       | 39(15)   | 51(14)   |
| C <sub>8</sub> H <sub>10</sub>                | 1,3-Dimethylbenzene                    | 106(58)                            | 91(93)    | 105(26)                       | 39(17)   | 51(14)   |
| C <sub>8</sub> H <sub>10</sub>                | 1,4-Dimethylbenzene                    | 106(52)                            | 91(85)    | 105(25)                       | 51(13)   | 39(13)   |
| C <sub>8</sub> H <sub>10</sub>                | Ethylbenzene                           | 106(45)                            | 91(146)   | 51(19)                        | 39(14)   | 65(12)   |
| F <sub>3</sub> N                              | Nitrogen trifluoride                   | 71(10)                             | 52(33)    | 33(13)                        | 14(3.0)  | 19(2.7)  |
| HCl                                           | Hydrogen chloride                      | 36(54)                             | 36(54)    | 38(17)                        | 35(9.2)  | 37(2.9)  |
| H <sub>2</sub> S                              | Hydrogen sulfide                       | 34(75)                             | 34(75)    | 32(33)                        | 33(32)   | 1(4.1)   |
| H <sub>3</sub> P                              | Ammonia                                | 17(32)                             | 17(32)    | 16(26)                        | 15(2.4)  | 14(0.7)  |
| H <sub>3</sub> N                              | Phosphine                              | 34(59)                             | 34(59)    | 33(20)                        | 31(19)   | 32(7.5)  |
| H <sub>4</sub> N <sub>2</sub>                 | Hydrazine                              | 32(48)                             | 32(48)    | 31(23)                        | 29(19)   | 30(15)   |
| NO                                            | Nitric oxide                           | 30(76)                             | 30(76)    | 14(5.7)                       | 15(1.8)  | 16(1.1)  |
| NO <sub>2</sub>                               | Nitrogen dioxide                       | 46(6.6)                            | 30(18)    | 16(4.0)                       | 14(1.7)  | 47(0.02) |
| N <sub>2</sub>                                | Nitrogen                               | 28(65)                             | 28(65)    | 14(3.3)                       | 29(0.47) | ...      |
| N <sub>2</sub> O                              | Nitrous oxide                          | 44(60)                             | 44(60)    | 30(19)                        | 14(7.8)  | 28(6.5)  |
| O <sub>2</sub>                                | Oxygen                                 | 32(54)                             | 32(54)    | 16(2.7)                       | 28(1.7)  | 34(0.22) |
| O <sub>2</sub> S                              | Sulfur dioxide                         | 64(47)                             | 64(47)    | 48(23)                        | 32(4.9)  | 16(2.4)  |

**Source:** L. Meites, ed., *Handbook of Analytical Chemistry*, McGraw-Hill, New York, 1963. J. A. Dean, ed., *Analytical Chemistry Handbook*, McGraw-Hill, New York, 1995.

---

# SECTION 8

---

## ELECTROLYTES, ELECTROMOTIVE FORCE, AND CHEMICAL EQUILIBRIUM

---

|                                                                                                                  |              |
|------------------------------------------------------------------------------------------------------------------|--------------|
| <b>8.1 ACTIVITY COEFFICIENTS</b>                                                                                 | <b>8.2</b>   |
| Table 8.1 Individual Activity Coefficients of Ions in Water at 25°C                                              | 8.3          |
| Table 8.2 Approximate Effective Ionic Radii in Aqueous Solutions at 25°C                                         | 8.4          |
| Table 8.3 Constants of the Debye-Hückel Equation from 0 to 100°C                                                 | 8.5          |
| Table 8.4 Individual Ionic Activity Coefficients at Higher Ionic Strengths at 25°C                               | 8.5          |
| <b>8.2 EQUILIBRIUM CONSTANTS</b>                                                                                 | <b>8.6</b>   |
| Table 8.5 Ionic Product Constant of Water                                                                        | 8.6          |
| Table 8.6 Solubility Product Constants                                                                           | 8.6          |
| <b>8.2.1 Proton-Transfer Reactions</b>                                                                           | <b>8.17</b>  |
| Table 8.7 Proton Transfer Reactions of Inorganic Materials in Water at 25°C                                      | 8.18         |
| Table 8.8 $pK_s$ Values of Organic Materials in Water at 25°C                                                    | 8.24         |
| Table 8.9 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures                             | 8.73         |
| Table 8.10 Properties of Common Acid-Base Solvents                                                               | 8.80         |
| Table 8.11 $pK_s$ Values for Proton-Transfer Reactions in Nonaqueous Solvents                                    | 8.81         |
| <b>8.2.2 Formation Constants of Metal Complexes</b>                                                              | <b>8.82</b>  |
| Table 8.12 Cumulative Formation Constants for Metal Complexes with Inorganic Ligands                             | 8.83         |
| Table 8.13 Cumulative Formation Constants for Metal Complexes with Organic Ligands                               | 8.88         |
| <b>8.3 BUFFER SOLUTIONS</b>                                                                                      | <b>8.104</b> |
| <b>8.3.1 Standard Reference pH Buffer Solutions</b>                                                              | <b>8.104</b> |
| Table 8.14 National Bureau of Standards (U.S.) Reference pH Buffer Solutions                                     | 8.105        |
| Table 8.15 Compositions of Standard pH Buffer Solutions [National Bureau of Standards (U.S.)]                    | 8.106        |
| <b>8.3.2 Standards for pH Measurement of Blood and Biological Media</b>                                          | <b>8.106</b> |
| Table 8.16 Composition and pH Values of Buffer Solutions                                                         | 8.107        |
| Table 8.17 Standard Reference Values $pH_s^*$ for the Measurement of Acidity in 50 Weight Percent Methanol-Water | 8.109        |
| Table 8.18 $pH^*$ Values for Buffer Solutions in Alcohol-Water Solvents at 25°C                                  | 8.109        |
| <b>8.3.3 Buffer Solutions Other Than Standards</b>                                                               | <b>8.110</b> |
| Table 8.19 pH Values of Biological and Other Buffers for Control Purposes                                        | 8.110        |
| <b>8.4 REFERENCE ELECTRODES</b>                                                                                  | <b>8.113</b> |
| Table 8.20 Potentials of Reference Electrodes in Volts as a Function of Temperature                              | 8.113        |
| Table 8.21 Potentials of Reference Electrodes (in Volts) at 25°C for Water–Organic Solvent Mixtures              | 8.114        |
| <b>8.4.1 Electrometric Measurement of pH</b>                                                                     | <b>8.115</b> |
| Table 8.22 Values of $2.3026RT/F$ at Several Temperatures                                                        | 8.115        |
| <b>8.5 INDICATORS</b>                                                                                            | <b>8.116</b> |
| Table 8.23 Indicators for Aqueous Acid-Base Titrations                                                           | 8.116        |
| Table 8.24 Mixed Indicators                                                                                      | 8.118        |

|            |                                                                                                                       |       |
|------------|-----------------------------------------------------------------------------------------------------------------------|-------|
| Table 8.25 | Fluorescent Indicators                                                                                                | 8.120 |
| Table 8.26 | Selected List of Oxidation-Reduction Indicators                                                                       | 8.122 |
| 8.6        | ELECTRODE POTENTIALS                                                                                                  | 8.124 |
| Table 8.27 | Potentials of the Elements and Their Compounds at 25°C                                                                | 8.124 |
| Table 8.28 | Potentials of Selected Half-Reactions at 25°C                                                                         | 8.137 |
| Table 8.29 | Overpotentials for Common Electrode Reactions at 25°C                                                                 | 8.140 |
| Table 8.30 | Half-Wave Potentials of Inorganic Materials                                                                           | 8.141 |
| Table 8.31 | Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C                                   | 8.146 |
| 8.7        | CONDUCTANCE                                                                                                           | 8.157 |
| Table 8.32 | Limiting Equivalent Ionic Conductances in Aqueous Solutions                                                           | 8.157 |
| Table 8.33 | Standard Solutions for Calibrating Conductivity Vessels                                                               | 8.160 |
| Table 8.34 | Electrical Conductivity of Various Pure Liquids                                                                       | 8.161 |
| Table 8.35 | Equivalent Conductivities of Electrolytes in Aqueous Solutions at 18°C                                                | 8.163 |
| Table 8.36 | Conductivity of Very Pure Water at Various Temperatures and the Equivalent Conductances of Hydrogen and Hydroxyl Ions | 8.168 |
| 8.7.1      | Common Conductance Relations                                                                                          | 8.168 |

8.1 ACTIVITY COEFFICIENTS

Although it is not possible to measure an individual ionic activity coefficient,  $f_i$ , it may be estimated from the following equation of the Debye-Hückel theory:

$$-\log f_i = \frac{Az_i^2\sqrt{I}}{1 + B\hat{a}\sqrt{I}}$$

where  $I$  is the ionic strength of the medium, and  $\hat{a}$  is the ion-size parameter—the effective ionic radius (Table 8.2). The values of  $A$  and  $B$  vary with the temperature and dielectric constant of the solvent; values from 0 to 100°C for aqueous medium ( $\hat{a}$  in angstrom units) are listed in Table 8.3. Corresponding values of  $A$  and  $B$  for unit weight of solvent (when employing molality) can be obtained by multiplying the corresponding values for unit volume (molarity units) by the square root of the density of water at the appropriate temperature.

The ionic strength can be estimated from the summation of the product molarity times ionic charge squared for all the ionic species present in the solution, i.e.,  $I = 0.5(c_1z_1^2 + c_2z_2^2 + \cdots + c_iz_i^2)$ .

Values for the activity coefficients of ions in water at 25°C are given in Table 8.1 in terms of their effective ionic radii.

At moderate ionic strengths a considerable improvement is effected by subtracting a term  $bI$  from the Debye-Hückel expression;  $b$  is an adjustable parameter which is 0.2 for water at 25°C. Table 8.4 gives the values of the ionic activity coefficients (for  $z_i$  from 1 to 6) with  $\hat{a}$  taken to be 4.6Å.

In general, the mean ionic activity coefficient is given by

$$f_{\pm} = {}^{(x+y)}\sqrt{f_+^x f_-^y}$$

**TABLE 8.1** Individual Activity Coefficients of Ions in Water at 25°C

| Effective Ionic Radii<br>$\bar{a}$ (in Å) | $f_i$ at Ionic Strength of |       |       |       |       |
|-------------------------------------------|----------------------------|-------|-------|-------|-------|
|                                           | 0.001                      | 0.005 | 0.01  | 0.05  | 0.1   |
| Univalent Ions                            |                            |       |       |       |       |
| 9                                         | 0.967                      | 0.933 | 0.914 | 0.86  | 0.83  |
| 8                                         | 0.966                      | 0.931 | 0.912 | 0.85  | 0.82  |
| 7                                         | 0.965                      | 0.930 | 0.909 | 0.845 | 0.81  |
| 6                                         | 0.965                      | 0.929 | 0.907 | 0.835 | 0.80  |
| 5                                         | 0.964                      | 0.928 | 0.904 | 0.83  | 0.79  |
| 4                                         | 0.964                      | 0.928 | 0.902 | 0.82  | 0.775 |
| 3.5                                       | 0.964                      | 0.926 | 0.900 | 0.81  | 0.76  |
| 3                                         | 0.964                      | 0.925 | 0.899 | 0.805 | 0.755 |
| 2.5                                       | 0.964                      | 0.924 | 0.898 | 0.80  | 0.75  |
| Divalent Ions                             |                            |       |       |       |       |
| 8                                         | 0.872                      | 0.755 | 0.69  | 0.52  | 0.45  |
| 7                                         | 0.872                      | 0.755 | 0.685 | 0.50  | 0.425 |
| 6                                         | 0.870                      | 0.749 | 0.675 | 0.485 | 0.405 |
| 5                                         | 0.868                      | 0.744 | 0.67  | 0.465 | 0.38  |
| 4.5                                       | 0.868                      | 0.741 | 0.663 | 0.45  | 0.36  |
| 4                                         | 0.867                      | 0.740 | 0.660 | 0.445 | 0.355 |
| Trivalent Ions                            |                            |       |       |       |       |
| 6                                         | 0.731                      | 0.52  | 0.415 | 0.195 | 0.13  |
| 5                                         | 0.728                      | 0.51  | 0.405 | 0.18  | 0.115 |
| 4                                         | 0.725                      | 0.505 | 0.395 | 0.16  | 0.095 |
| Tetravalent Ions                          |                            |       |       |       |       |
| 11                                        | 0.588                      | 0.35  | 0.255 | 0.10  | 0.065 |
| 5                                         | 0.57                       | 0.31  | 0.20  | 0.048 | 0.021 |
| Pentavalent Ions                          |                            |       |       |       |       |
| 9                                         | 0.43                       | 0.18  | 0.105 | 0.020 | 0.009 |

where  $f_+$ ,  $f_-$  are the individual ionic activity coefficients, and  $x, y$  are the charge numbers ( $z_+$ ,  $z_-$ ) of the respective ions. In binary electrolyte solution.

$$f_{\pm} = \sqrt{f_+ f_-}$$

In ternary electrolytes, e.g.,  $\text{BaCl}_2$  or  $\text{K}_2\text{SO}_4$ ,

$$f_{\pm} = \sqrt[3]{f_+ f_-^2} \quad \text{or} \quad f_{\pm} = \sqrt[3]{f_+^2 f_-}$$

In quaternary electrolytes, e.g.,  $\text{LaCl}_3$  or  $\text{K}_3[\text{Fe}(\text{CN})_6]$ ,

$$f_{\pm} = \sqrt[4]{f_+ f_-^3} \quad \text{or} \quad f_{\pm} = \sqrt[4]{f_+^3 f_-}$$

**TABLE 8.2** Approximate Effective Ionic Radii in Aqueous Solutions at 25°C

| $\text{\AA}$ (in $\text{\AA}$ ) | Inorganic Ions                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | $\text{\AA}$ (in $\text{\AA}$ ) | Organic Ions                                                                                                                                                                                                                                                                                                                                                                                                          |
|---------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 2.5.....                        | Rb <sup>+</sup> , Cs <sup>+</sup> , NH <sub>4</sub> <sup>+</sup> , Tl <sup>+</sup> , Ag <sup>+</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 3.5.....                        | HCOO <sup>-</sup> , H <sub>2</sub> Cit <sup>-</sup> , CH <sub>3</sub> NH <sub>3</sub> <sup>+</sup> , (CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> <sup>+</sup>                                                                                                                                                                                                                                                     |
| 3.....                          | K <sup>+</sup> , Cl <sup>-</sup> , Br <sup>-</sup> , I <sup>-</sup> , CN <sup>-</sup> , NO <sub>2</sub> <sup>-</sup> , NO <sub>3</sub> <sup>-</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 4.....                          | H <sub>3</sub> N <sup>+</sup> CH <sub>2</sub> COOH, (CH <sub>3</sub> ) <sub>3</sub> NH <sup>+</sup> , C <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> <sup>+</sup>                                                                                                                                                                                                                                                      |
| 3.5.....                        | OH <sup>-</sup> , F <sup>-</sup> , SCN <sup>-</sup> , OCN <sup>-</sup> , HS <sup>-</sup> , ClO <sub>3</sub> <sup>-</sup> , ClO <sub>4</sub> <sup>-</sup> , BrO <sub>3</sub> <sup>-</sup> , IO <sub>4</sub> <sup>-</sup> , MnO <sub>4</sub> <sup>-</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 4.5.....                        | CH <sub>3</sub> COO <sup>-</sup> , ClCH <sub>2</sub> COO <sup>-</sup> , (CH <sub>3</sub> ) <sub>4</sub> N <sup>+</sup> , (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH <sub>2</sub> <sup>+</sup> ,<br>H <sub>2</sub> NCH <sub>2</sub> COO <sup>-</sup> , oxalate <sup>2-</sup> , HCit <sup>2-</sup>                                                                                                                |
| 4.....                          | Na <sup>+</sup> , CdCl <sup>+</sup> , Hg <sub>2</sub> <sup>2+</sup> , ClO <sub>2</sub> <sup>-</sup> , IO <sub>3</sub> <sup>-</sup> , HCO <sub>3</sub> <sup>-</sup> , H <sub>2</sub> PQ <sup>-</sup> , HSQ <sup>-</sup> ,<br>H <sub>2</sub> AsO <sub>4</sub> <sup>-</sup> , SO <sub>4</sub> <sup>2-</sup> , S <sub>2</sub> O <sub>3</sub> <sup>2-</sup> , S <sub>2</sub> O <sub>8</sub> <sup>2-</sup> , SeO <sub>4</sub> <sup>2-</sup> , CrO <sub>4</sub> <sup>2-</sup> , HPO <sub>4</sub> <sup>2-</sup> , S <sub>2</sub> O <sub>6</sub> <sup>2-</sup> ,<br>PO <sub>4</sub> <sup>3-</sup> , Fe(CN) <sub>6</sub> <sup>3-</sup> , Cr(NH <sub>3</sub> ) <sub>6</sub> <sup>3+</sup> , Co(NH <sub>3</sub> ) <sub>6</sub> <sup>3+</sup> , Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O <sup>3+</sup> | 5.....                          | Cl <sub>2</sub> CHCOO <sup>-</sup> , Cl <sub>3</sub> COO <sup>-</sup> , (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> NH <sup>+</sup> , C <sub>3</sub> H <sub>7</sub> NH <sub>3</sub> <sup>+</sup> , Cit <sup>3-</sup> , succi-<br>nate <sup>2-</sup> , malonate <sup>2-</sup> , tartrate <sup>2-</sup>                                                                                                               |
| 4.5.....                        | Pb <sup>2+</sup> , CO <sub>3</sub> <sup>2-</sup> , SO <sub>3</sub> <sup>2-</sup> , MoO <sub>4</sub> <sup>2-</sup> , Co(NH <sub>3</sub> ) <sub>5</sub> Cl <sup>2+</sup> , Fe(CN) <sub>5</sub> NO <sup>2-</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 6.....                          | benzoate <sup>-</sup> , hydroxybenzoate <sup>-</sup> , chlorobenzoate <sup>-</sup> , phenylace-<br>tate <sup>-</sup> , vinylacetate <sup>-</sup> , (CH <sub>3</sub> ) <sub>2</sub> C=CHCOO <sup>-</sup> , (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> N <sup>+</sup> ,<br>(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH <sub>2</sub> , phthalate <sup>2-</sup> , glutarate <sup>2-</sup> , adipate <sup>2-</sup> |
| 5.....                          | Sr <sup>2+</sup> , Ba <sup>2+</sup> , Ra <sup>2+</sup> , Cd <sup>2+</sup> , Hg <sup>2+</sup> , S <sup>2-</sup> , S <sub>2</sub> O <sub>4</sub> <sup>2-</sup> , WO <sub>4</sub> <sup>2-</sup> , Fe(CN) <sub>6</sub> <sup>4-</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 7.....                          | trinitrophenolate <sup>-</sup> , (C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> NH <sup>+</sup> , methoxybenzoate <sup>-</sup> , pime-<br>late <sup>2-</sup> , suberate <sup>2-</sup> , Congo red anion <sup>2-</sup>                                                                                                                                                                                                  |
| 6.....                          | Li <sup>+</sup> , Ca <sup>2+</sup> , Cu <sup>2+</sup> , Zn <sup>2+</sup> , Sn <sup>2+</sup> , Mn <sup>2+</sup> , Fe <sup>2+</sup> , Ni <sup>2+</sup> , Co <sup>2+</sup> , Co(en) <sub>3</sub> <sup>3+</sup> ,<br>Co(S <sub>2</sub> O <sub>3</sub> )(CN) <sub>5</sub> <sup>4-</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 8.....                          | (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> CHCOO <sup>-</sup> , (C <sub>3</sub> H <sub>7</sub> ) <sub>4</sub> N <sup>+</sup>                                                                                                                                                                                                                                                                                       |
| 8.....                          | Mg <sup>2+</sup> , Be <sup>2+</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                 |                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 9.....                          | H <sup>+</sup> , Al <sup>3+</sup> , Fe <sup>3+</sup> , Cr <sup>3+</sup> , Sc <sup>3+</sup> , Y <sup>3+</sup> , La <sup>3+</sup> , In <sup>3+</sup> , Ce <sup>3+</sup> , Pr <sup>3+</sup> , Nd <sup>3+</sup> ,<br>Sm <sup>3+</sup> , Co(SO <sub>3</sub> ) <sub>2</sub> (CN) <sub>5</sub> <sup>5-</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                 |                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 11.....                         | Th <sup>4+</sup> , Zr <sup>4+</sup> , Ce <sup>4+</sup> , Sn <sup>4+</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                 |                                                                                                                                                                                                                                                                                                                                                                                                                       |

**TABLE 8.3** Constants of the Debye-Hückel Equation from 0 to 100°C

$$-\log f_i = \frac{Az_i^2\sqrt{I}}{1 + B\hat{a}\sqrt{I}}$$

| Temp.,<br>°C | Unit Volume of Solvent |        | Temp.,<br>°C | Unit Volume of Solvent |        |
|--------------|------------------------|--------|--------------|------------------------|--------|
|              | A                      | B      |              | A                      | B      |
| 0            | 0.4918                 | 0.3248 | 55           | 0.5432                 | 0.3358 |
| 5            | 0.4952                 | 0.3256 | 60           | 0.5494                 | 0.3371 |
| 10           | 0.4989                 | 0.3264 | 65           | 0.5558                 | 0.3384 |
| 15           | 0.5028                 | 0.3273 | 70           | 0.5625                 | 0.3397 |
| 20           | 0.5070                 | 0.3282 | 75           | 0.5695                 | 0.3411 |
| 25           | 0.5115                 | 0.3291 | 80           | 0.5767                 | 0.3426 |
| 30           | 0.5161                 | 0.3301 | 85           | 0.5842                 | 0.3440 |
| 35           | 0.5211                 | 0.3312 | 90           | 0.5920                 | 0.3456 |
| 40           | 0.5262                 | 0.3323 | 95           | 0.6001                 | 0.3471 |
| 45           | 0.5317                 | 0.3334 | 100          | 0.6086                 | 0.3488 |
| 50           | 0.5373                 | 0.3346 |              |                        |        |

The values for unit weight of solvent (molality scale) can be obtained by multiplying the corresponding values for unit volume by the square root of the density of water at the appropriate temperature.

**TABLE 8.4** Individual Ionic Activity Coefficients at Higher Ionic Strengths at 25°C

The values were calculated from the modified Debye-Hückel equation utilizing the modifications proposed by Robinson and by Guggenheim and Bates:

$$-\frac{\log f_i}{z_i^2} = \frac{0.511I}{1 + 1.5I} - 0.2I$$

where  $I$  is the ionic strength and  $\hat{a}$  is assumed to be 4.6 Å.

| $I$  | $-\frac{\log_{10} f_i}{z_i^2}$ | $f_i$ for $z_i =$ |       |                    |        |                     |          |
|------|--------------------------------|-------------------|-------|--------------------|--------|---------------------|----------|
|      |                                | 1                 | 2     | 3                  | 4      | 5                   | 6        |
| 0.05 | 0.0756                         | 0.840             | 0.498 | 0.209              | 0.0617 | 0.0129              | 0.00190  |
| 0.1  | 0.0896                         | 0.814             | 0.438 | 0.156              | 0.0369 | 0.00576             | 0.000595 |
| 0.2  | 0.0968                         | 0.800             | 0.410 | 0.138              | 0.0283 | 0.00380             | 0.000328 |
| 0.3  | 0.0936                         | 0.806             | 0.422 | 0.144              | 0.0318 | 0.00457             | 0.000427 |
| 0.4  | 0.0858                         | 0.821             | 0.454 | 0.169              | 0.0424 | 0.00716             | 0.000815 |
| 0.5  | 0.0753                         | 0.841             | 0.500 | 0.210              | 0.0624 | 0.0131              | 0.00195  |
| 0.6  | 0.0631                         | 0.865             | 0.559 | 0.270 <sub>5</sub> | 0.0978 | 0.0265              | 0.00535  |
| 0.7  | 0.0496                         | 0.892             | 0.633 | 0.358              | 0.161  | 0.0575 <sub>5</sub> | 0.0164   |
| 0.8  | 0.0352                         | 0.922             | 0.723 | 0.482              | 0.273  | 0.132               | 0.0541   |
| 0.9  | 0.0201                         | 0.955             | 0.831 | 0.659              | 0.477  | 0.314               | 0.189    |
| 1.0  | 0.0044                         | 0.900             | 0.960 | 0.913              | 0.850  | 0.776               | 0.694    |

8.2 EQUILIBRIUM CONSTANTS

TABLE 8.5 Ionic Product Constant of Water

This table gives values of pKw on a molal scale, where Kw is the ionic activity product constant of water. Values are from W. L. Marshall and E. U. Franck, *J. Phys. Chem. Ref. Data*, **10**:295 (1981).

| Temp.,<br>°C | pKw    | Temp.,<br>°C | pKw    | Temp.,<br>°C | pKw    |
|--------------|--------|--------------|--------|--------------|--------|
| 0            | 14.938 | 45           | 13.405 | 95           | 12.345 |
| 5            | 14.727 | 50           | 13.275 | 100          | 12.264 |
| 10           | 14.528 | 55           | 13.152 | 125          | 11.911 |
| 15           | 14.340 | 60           | 13.034 | 150          | 11.637 |
| 18           | 14.233 | 65           | 12.921 | 175          | 11.431 |
| 20           | 14.163 | 70           | 12.814 | 200          | 11.288 |
| 25           | 13.995 | 75           | 12.711 | 225          | 11.207 |
| 30           | 13.836 | 80           | 12.613 | 250          | 11.192 |
| 35           | 13.685 | 85           | 12.520 | 275          | 11.251 |
| 40           | 13.542 | 90           | 12.431 | 300          | 11.406 |

TABLE 8.6 Solubility Product Constants

The data refer to various temperatures between 18 and 25°C, and were compiled from values cited by Bjerrum, Schwarzenbach, and Sillen, *Stability Constants of Metal Complexes*, part II, Chemical Society, London, 1958, and values taken from publications of the IUPAC Solubility Data Project: *Solubility Data Series*, International Union of Pure and Applied Chemistry, Pergamon Press, Oxford, 1979–1992; H. L. Clever, and F. J. Johnston, *J. Phys. Chem. Ref. Data*, **9**:751 (1980); Y. Marcus, *Ibid.* **9**:1307 (1980); H. L. Clever, S. A. Johnson, and M. E. Derrick, *Ibid.* **14**:631 (1985), and **21**:941 (1992).

In the table, “L” is the abbreviation of the organic ligand.

| Compound                     | Formula                                          | pK <sub>sp</sub> | K <sub>sp</sub>          |
|------------------------------|--------------------------------------------------|------------------|--------------------------|
| Actinium<br>hydroxide        | Ac(OH) <sub>3</sub>                              | 15               | 1 × 10 <sup>−15</sup>    |
| Aluminum<br>arsonate         | AlAsO <sub>4</sub>                               | 15.80            | 1.6 × 10 <sup>−16</sup>  |
| cupferrate                   | AlL <sub>3</sub>                                 | 18.64            | 2.3 × 10 <sup>−19</sup>  |
| hydroxide                    | Al(OH) <sub>3</sub>                              | 32.89            | 1.3 × 10 <sup>−33</sup>  |
| phosphate                    | AlPO <sub>4</sub>                                | 20.01            | 9.84 × 10 <sup>−21</sup> |
| 8-quinolinolate              | AlL <sub>3</sub>                                 | 29.00            | 1.00 × 10 <sup>−29</sup> |
| selenide                     | Al <sub>2</sub> Se <sub>3</sub>                  | 24.4             | 4 × 10 <sup>−25</sup>    |
| sulfide                      | Al <sub>2</sub> S <sub>3</sub>                   | 6.7              | 2 × 10 <sup>−7</sup>     |
| Americium<br>(III) hydroxide | Am(OH) <sub>3</sub>                              | 19.57            | 2.7 × 10 <sup>−20</sup>  |
| (IV) hydroxide               | Am(OH) <sub>4</sub>                              | 56               | 1 × 10 <sup>−56</sup>    |
| Ammonium<br>uranyl arsenate  | NH <sub>4</sub> UO <sub>2</sub> AsO <sub>4</sub> | 23.77            | 1.7 × 10 <sup>−24</sup>  |
| Arsenic<br>(III) sulfide     | As <sub>2</sub> S <sub>3</sub>                   | 21.68            | 2.1 × 10 <sup>−22</sup>  |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound               | Formula                      | $pK_{sp}$ | $K_{sp}$               |
|------------------------|------------------------------|-----------|------------------------|
| Barium                 |                              |           |                        |
| arsenate               | $Ba_3(AsO_4)_2$              | 50.11     | $8.0 \times 10^{-51}$  |
| bromate                | $Ba(BrO_3)_2$                | 5.50      | $2.43 \times 10^{-4}$  |
| carbonate              | $BaCO_3$                     | 8.59      | $2.58 \times 10^{-9}$  |
| chromate               | $BaCrO_4$                    | 9.93      | $1.17 \times 10^{-10}$ |
| ferricyanide 6-hydrate | $Ba_2[Fe(CN)_6] \cdot 6H_2O$ | 7.49      | $3.2 \times 10^{-8}$   |
| fluoride               | $BaF_2$                      | 6.74      | $1.84 \times 10^{-7}$  |
| hexafluorosilicate     | $BaSiF_6$                    | 6         | $1 \times 10^{-6}$     |
| hydrogen phosphate     | $BaHPO_4$                    | 6.49      | $3.2 \times 10^{-7}$   |
| hydroxide 8-hydrate    | $Ba(OH)_2 \cdot 8H_2O$       | 3.59      | $2.55 \times 10^{-4}$  |
| iodate hydrate         | $Ba(IO_3)_2 \cdot H_2O$      | 8.40      | $4.01 \times 10^{-9}$  |
| molybdate              | $BaMoO_4$                    | 7.45      | $3.54 \times 10^{-8}$  |
| niobate                | $Ba(NbO_3)_2$                | 16.50     | $3.2 \times 10^{-17}$  |
| nitrate                | $Ba(NO_3)_2$                 | 2.33      | $4.64 \times 10^{-3}$  |
| oxalate                | $BaC_2O_4$                   | 6.79      | $1.6 \times 10^{-7}$   |
| oxalate hydrate        | $BaC_2O_4 \cdot H_2O$        | 7.64      | $2.3 \times 10^{-8}$   |
| permanganate           | $Ba(MnO_4)_2$                | 9.61      | $2.5 \times 10^{-10}$  |
| perrhenate             | $Ba(ReO_4)_2$                | 1.28      | $5.2 \times 10^{-2}$   |
| phosphate              | $Ba_3(PO_4)_2$               | 22.47     | $3.4 \times 10^{-23}$  |
| pyrophosphate          | $Ba_2P_2O_7$                 | 10.50     | $3.2 \times 10^{-11}$  |
| 8-quinolinolate        | $BaL_2$                      | 8.30      | $5.0 \times 10^{-9}$   |
| selenate               | $BaSeO_4$                    | 7.47      | $3.40 \times 10^{-8}$  |
| sulfate                | $BaSO_4$                     | 9.97      | $1.08 \times 10^{-10}$ |
| sulfite                | $BaSO_3$                     | 9.30      | $5.0 \times 10^{-10}$  |
| thiosulfate            | $BaS_2O_3$                   | 4.79      | $1.6 \times 10^{-5}$   |
| Beryllium              |                              |           |                        |
| carbonate 4-hydrate    | $BeCO_3 \cdot 4H_2O$         | 3         | $1 \times 10^{-3}$     |
| hydroxide (amorphous)  | $Be(OH)_2$                   | 21.16     | $6.92 \times 10^{-22}$ |
| molybdate              | $BeMoO_4$                    | 1.49      | $3.2 \times 10^{-2}$   |
| niobate                | $Be(NbO_3)_2$                | 15.92     | $1.2 \times 10^{-16}$  |
| Bismuth                |                              |           |                        |
| arsenate               | $BiAsO_4$                    | 9.35      | $4.43 \times 10^{-10}$ |
| cupferrate             | $BiL_3$                      | 27.22     | $6.0 \times 10^{-28}$  |
| hydroxide              | $Bi(OH)_3$                   | 30.4      | $6.0 \times 10^{-31}$  |
| iodide                 | $BiI_3$                      | 18.11     | $7.71 \times 10^{-19}$ |
| oxide bromide          | $BiOBr$                      | 6.52      | $3.0 \times 10^{-7}$   |
| oxide chloride         | $BiOCl$                      | 30.75     | $1.8 \times 10^{-31}$  |
| oxide hydroxide        | $BiO(OH)$                    | 9.4       | $4 \times 10^{-10}$    |
| oxide nitrate          | $BiO(NO_3)$                  | 2.55      | $2.82 \times 10^{-3}$  |
| oxide nitrite          | $BiO(NO_2)$                  | 6.31      | $4.9 \times 10^{-7}$   |
| oxide thiocyanate      | $BiO(SCN)$                   | 6.80      | $1.6 \times 10^{-7}$   |
| phosphate              | $BiPO_4$                     | 22.89     | $1.3 \times 10^{-23}$  |
| sulfide                | $Bi_2S_3$                    | 97        | $1 \times 10^{-97}$    |
| Cadmium                |                              |           |                        |
| anthranilate           | $CdL_2$                      | 8.27      | $5.4 \times 10^{-9}$   |
| arsenate               | $Cd_3(AsO_4)_2$              | 32.66     | $2.2 \times 10^{-33}$  |
| benzoate 2-hydrate     | $CdL_2 \cdot 2H_2O$          | 2.7       | $2 \times 10^{-3}$     |
| borate, <i>meta</i>    | $Cd(BO_2)_2$                 | 8.64      | $2.3 \times 10^{-9}$   |
| carbonate              | $CdCO_3$                     | 12.0      | $1.0 \times 10^{-12}$  |
| cyanide                | $Cd(CN)_2$                   | 8.0       | $1.0 \times 10^{-8}$   |
| ferrocyanide           | $Cd_2[Fe(CN)_6]$             | 16.49     | $3.2 \times 10^{-17}$  |
| fluoride               | $CdF_2$                      | 2.19      | $6.44 \times 10^{-3}$  |



**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound                | Formula                      | $pK_{sp}$ | $K_{sp}$               |
|-------------------------|------------------------------|-----------|------------------------|
| hydroxide               | $Cd(OH)_2$ fresh             | 14.14     | $7.2 \times 10^{-15}$  |
| iodate                  | $Cd(IO_3)_2$                 | 7.60      | $2.5 \times 10^{-8}$   |
| oxalate 3-water         | $CdC_2O_4 \cdot 3H_2O$       | 7.85      | $1.42 \times 10^{-8}$  |
| phosphate               | $Cd_3(PO_4)_2$               | 32.60     | $2.53 \times 10^{-33}$ |
| quinaldate              | $CdL_2$                      | 12.30     | $5.0 \times 10^{-13}$  |
| sulfide                 | $CdS$                        | 26.10     | $8.0 \times 10^{-27}$  |
| tungstate               | $CdWO_4$                     | 5.7       | $2 \times 10^{-6}$     |
| <b>Calcium</b>          |                              |           |                        |
| acetate 3-water         | $Ca(OAc)_2 \cdot 3H_2O$      | 2.4       | $4 \times 10^{-3}$     |
| arsenate                | $Ca_3(AsO_4)_2$              | 18.17     | $6.8 \times 10^{-19}$  |
| benzoate 3-water        | $CaL_2 \cdot 3H_2O$          | 2.4       | $4 \times 10^{-3}$     |
| carbonate               | $CaCO_3$                     | 8.54      | $2.8 \times 10^{-9}$   |
| carbonate (calcite)     | $CaCO_3$                     | 8.47      | $3.36 \times 10^{-9}$  |
| carbonate (aragonite)   | $CaCO_3$                     | 8.22      | $6.0 \times 10^{-9}$   |
| carbonatomagnesium      | $Ca[Mg(CO_3)_2]$ dolomite    | 11        | $1 \times 10^{-11}$    |
| chromate                | $CaCrO_4$                    | 3.15      | $7.1 \times 10^{-4}$   |
| fluoride                | $CaF_2$                      | 8.28      | $5.3 \times 10^{-9}$   |
| hexafluorosilicate      | $Ca[SiF_6]$                  | 3.09      | $8.1 \times 10^{-4}$   |
| hydrogen phosphate      | $CaHPO_4$                    | 7.0       | $1.0 \times 10^{-7}$   |
| hydroxide               | $Ca(OH)_2$                   | 5.26      | $5.5 \times 10^{-6}$   |
| iodate 6-water          | $Ca(IO_3)_2 \cdot 6H_2O$     | 6.15      | $7.10 \times 10^{-7}$  |
| molybdate               | $CaMoO_4$                    | 7.84      | $1.46 \times 10^{-8}$  |
| niobate                 | $Ca(NbO_3)_2$                | 17.06     | $8.7 \times 10^{-18}$  |
| oxalate hydrate         | $CaC_2O_4 \cdot H_2O$        | 8.63      | $2.32 \times 10^{-9}$  |
| phosphate               | $Ca_3(PO_4)_2$               | 28.68     | $2.07 \times 10^{-29}$ |
| 8-quinolinolate         | $CaL_2$                      | 11.12     | $7.6 \times 10^{-12}$  |
| selenate                | $CaSeO_4$                    | 3.09      | $8.1 \times 10^{-4}$   |
| selenite                | $CaSeO_3$                    | 5.53      | $8.0 \times 10^{-6}$   |
| silicate, <i>meta</i>   | $CaSiO_3$                    | 7.60      | $2.5 \times 10^{-8}$   |
| sulfate                 | $CaSO_4$                     | 4.31      | $4.93 \times 10^{-5}$  |
| sulfate dihydrate       | $CaSO_4 \cdot 2H_2O$         | 4.50      | $3.14 \times 10^{-5}$  |
| sulfite                 | $CaSO_3$                     | 7.17      | $6.8 \times 10^{-8}$   |
| sulfite 0.5-water       | $CaSO_3 \cdot 0.5H_2O$       | 6.51      | $3.1 \times 10^{-7}$   |
| tartrate dihydrate      | $CaL \cdot 2H_2O$            | 6.11      | $7.7 \times 10^{-7}$   |
| tungstate               | $CaWO_4$                     | 8.06      | $8.7 \times 10^{-9}$   |
| <b>Cerium</b>           |                              |           |                        |
| (III) fluoride          | $CeF_3$                      | 15.1      | $8 \times 10^{-16}$    |
| (III) hydroxide         | $Ce(OH)_3$                   | 19.80     | $1.6 \times 10^{-20}$  |
| (IV) hydroxide          | $Ce(OH)_4$                   | 47.7      | $2 \times 10^{-48}$    |
| (III) iodate            | $Ce(IO_3)_3$                 | 9.50      | $3.2 \times 10^{-10}$  |
| (IV) iodate             | $Ce(IO_3)_4$                 | 16.3      | $5 \times 10^{-17}$    |
| (III) oxalate 9-water   | $Ce_2(C_2O_4)_3 \cdot 9H_2O$ | 25.50     | $3.2 \times 10^{-26}$  |
| (III) phosphate         | $CePO_4$                     | 23        | $1 \times 10^{-23}$    |
| (III) selenite          | $Ce_2(SeO_3)_3$              | 24.43     | $3.7 \times 10^{-25}$  |
| (III) sulfide           | $Ce_2S_3$                    | 10.22     | $6.0 \times 10^{-11}$  |
| (III) tartrate          | $Ce_2L_3$                    | 19.0      | $1.0 \times 10^{-19}$  |
| <b>Cesium</b>           |                              |           |                        |
| bromate                 | $CsBrO_3$                    | 1.7       | $5 \times 10^{-2}$     |
| chlorate                | $CsClO_3$                    | 1.4       | $4 \times 10^{-2}$     |
| cobaltihexanitrite      | $Cs_3[Co(NO_2)_6]$           | 15.24     | $5.7 \times 10^{-16}$  |
| hexachloroplatinate(IV) | $Cs_2[PtCl_6]$               | 7.50      | $3.2 \times 10^{-8}$   |
| hexafluoroplatinate(IV) | $Cs_2[PtF_6]$                | 5.62      | $2.4 \times 10^{-6}$   |
| hexafluorosilicate      | $Cs_2[SiF_6]$                | 4.90      | $1.3 \times 10^{-5}$   |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound           | Formula                    | $pK_{sp}$ | $K_{sp}$               |
|--------------------|----------------------------|-----------|------------------------|
| perchlorate        | $CsClO_4$                  | 2.40      | $3.95 \times 10^{-3}$  |
| periodate          | $CsIO_4$                   | 5.29      | $5.16 \times 10^{-6}$  |
| permanganate       | $CsMnO_4$                  | 4.08      | $8.2 \times 10^{-5}$   |
| perrhanate         | $CsReO_4$                  | 3.40      | $4.0 \times 10^{-4}$   |
| tetrafluoroborate  | $Cs[BF_4]$                 | 4.7       | $5 \times 10^{-5}$     |
| Chromium(II)       |                            |           |                        |
| hydroxide          | $Cr(OH)_2$                 | 15.7      | $2 \times 10^{-16}$    |
| Chromium(III)      |                            |           |                        |
| arsenate           | $CrAsO_4$                  | 20.11     | $7.7 \times 10^{-21}$  |
| fluoride           | $CrF_3$                    | 10.18     | $6.6 \times 10^{-11}$  |
| hydroxide          | $Cr(OH)_3$                 | 30.20     | $6.3 \times 10^{-31}$  |
| phosphate 4-water  | $CrPO_4 \cdot 4H_2O$ green | 22.62     | $2.4 \times 10^{-23}$  |
|                    | violet                     | 17.00     | $1.0 \times 10^{-17}$  |
| Cobalt             |                            |           |                        |
| anthranilate       | $CoL_2$                    | 9.68      | $2.1 \times 10^{-10}$  |
| arsenate           | $Co_3(AsO_4)_2$            | 28.17     | $6.80 \times 10^{-29}$ |
| carbonate          | $CoCO_3$                   | 12.84     | $1.4 \times 10^{-13}$  |
| ferrocyanide       | $Co_2[Fe(CN)_6]$           | 14.74     | $1.8 \times 10^{-15}$  |
| hydrogen phosphate | $CoHPO_4$                  | 6.7       | $2 \times 10^{-7}$     |
| (II) hydroxide     | $Co(OH)_2$ fresh           | 14.23     | $5.92 \times 10^{-15}$ |
| (III) hydroxide    | $Co(OH)_3$                 | 43.80     | $1.6 \times 10^{-44}$  |
| iodate             | $Co(IO_3)_2$               | 4.0       | $1.0 \times 10^{-4}$   |
| phosphate          | $Co_3(PO_4)_2$             | 34.69     | $2.05 \times 10^{-35}$ |
| selenite           | $CoSeO_3$                  | 6.80      | $1.6 \times 10^{-7}$   |
| quinaldate         | $CoL_2$                    | 10.80     | $1.6 \times 10^{-11}$  |
| 8-quinolinolate    | $CoL_2$                    | 24.80     | $1.6 \times 10^{-25}$  |
| sulfide            | $\alpha$ -CoS              | 20.40     | $4.0 \times 10^{-21}$  |
|                    | $\beta$ -CoS               | 24.70     | $2.0 \times 10^{-25}$  |
| Copper(I)          |                            |           |                        |
| azide              | $CuN_3$                    | 8.31      | $4.9 \times 10^{-9}$   |
| bromide            | $CuBr$                     | 8.20      | $6.27 \times 10^{-9}$  |
| chloride           | $CuCl$                     | 6.76      | $1.72 \times 10^{-7}$  |
| cyanide            | $CuCN$                     | 19.46     | $3.47 \times 10^{-20}$ |
| hydroxide          | $CuOH$                     | 14        | $1 \times 10^{-14}$    |
| iodide             | $CuI$                      | 11.90     | $1.27 \times 10^{-12}$ |
| sulfide            | $Cu_2S$                    | 47.60     | $2.5 \times 10^{-48}$  |
| tetraphenylborate  | $CuL$                      | 8.0       | $1.0 \times 10^{-8}$   |
| thiocyanate        | $CuSCN$                    | 12.75     | $1.77 \times 10^{-13}$ |
| Copper(II)         |                            |           |                        |
| anthranilate       | $CuL_2$                    | 13.22     | $6.0 \times 10^{-14}$  |
| arsenate           | $Cu_3(AsO_4)_2$            | 35.10     | $7.95 \times 10^{-36}$ |
| azide              | $Cu(N_3)_2$                | 9.20      | $6.3 \times 10^{-10}$  |
| carbonate          | $CuCO_3$                   | 9.86      | $1.4 \times 10^{-10}$  |
| chromate           | $CuCrO_4$                  | 5.44      | $3.6 \times 10^{-6}$   |
| dithiooxamide      | $CuL$                      | 15.12     | $7.67 \times 10^{-16}$ |
| ferrocyanide       | $Cu_2[Fe(CN)_6]$           | 15.89     | $1.3 \times 10^{-16}$  |
| hydroxide          | $Cu(OH)_2$                 | 19.66     | $2.2 \times 10^{-20}$  |
| iodate             | $Cu(IO_3)_2$               | 7.16      | $6.94 \times 10^{-8}$  |
| oxalate            | $CuC_2O_4$                 | 9.35      | $4.43 \times 10^{-10}$ |
| phosphate          | $Cu_3(PO_4)_2$             | 36.85     | $1.40 \times 10^{-37}$ |
| pyrophosphate      | $Cu_3P_2O_7$               | 15.08     | $8.3 \times 10^{-16}$  |
| quinaldate         | $CuL_2$                    | 16.80     | $1.6 \times 10^{-17}$  |
| 8-quinolinolate    | $CuL_2$                    | 29.70     | $2.0 \times 10^{-30}$  |

TABLE 8.6 Solubility Product Constants (Continued)

| Compound            | Formula                                                               | pK <sub>sp</sub> | K <sub>sp</sub>          |
|---------------------|-----------------------------------------------------------------------|------------------|--------------------------|
| selenite            | CuSeO <sub>3</sub>                                                    | 7.68             | 2.1 × 10 <sup>-8</sup>   |
| sulfide             | CuS                                                                   | 35.20            | 6.3 × 10 <sup>-36</sup>  |
| Dysprosium          |                                                                       |                  |                          |
| chromate 10-water   | Dy <sub>2</sub> (CrO <sub>4</sub> ) <sub>3</sub> · 10H <sub>2</sub> O | 8                | 1 × 10 <sup>-8</sup>     |
| hydroxide           | Dy(OH) <sub>3</sub>                                                   | 21.85            | 1.4 × 10 <sup>-22</sup>  |
| Erbium              |                                                                       |                  |                          |
| hydroxide           | Er(OH) <sub>3</sub>                                                   | 23.39            | 4.1 × 10 <sup>-24</sup>  |
| Europium            |                                                                       |                  |                          |
| hydroxide           | Eu(OH) <sub>3</sub>                                                   | 23.03            | 9.38 × 10 <sup>-24</sup> |
| Gadolinium          |                                                                       |                  |                          |
| hydrogen carbonate  | Gd(HCO <sub>3</sub> ) <sub>3</sub>                                    | 1.7              | 2 × 10 <sup>-2</sup>     |
| hydroxide           | Gd(OH) <sub>3</sub>                                                   | 22.74            | 1.8 × 10 <sup>-23</sup>  |
| Gallium             |                                                                       |                  |                          |
| ferrocyanide        | Ga <sub>4</sub> [Fe(CN) <sub>6</sub> ] <sub>3</sub>                   | 33.82            | 1.5 × 10 <sup>-34</sup>  |
| hydroxide           | Ga(OH) <sub>3</sub>                                                   | 35.14            | 7.28 × 10 <sup>-36</sup> |
| 8-quinolinolate     | GaL <sub>3</sub>                                                      | 40.80            | 1.6 × 10 <sup>-41</sup>  |
| Germanium           |                                                                       |                  |                          |
| oxide               | GeO <sub>2</sub>                                                      | 57.0             | 1.0 × 10 <sup>-57</sup>  |
| Gold(I)             |                                                                       |                  |                          |
| chloride            | AuCl                                                                  | 12.70            | 2.0 × 10 <sup>-13</sup>  |
| iodide              | AuI                                                                   | 22.80            | 1.6 × 10 <sup>-23</sup>  |
| Gold(III)           |                                                                       |                  |                          |
| chloride            | AuCl <sub>3</sub>                                                     | 24.50            | 3.2 × 10 <sup>-25</sup>  |
| hydroxide           | Au(OH) <sub>3</sub>                                                   | 45.26            | 5.5 × 10 <sup>-46</sup>  |
| iodide              | AuI <sub>3</sub>                                                      | 46               | 1 × 10 <sup>-46</sup>    |
| oxalate             | Au <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>         | 10               | 1 × 10 <sup>-10</sup>    |
| Hafnium             |                                                                       |                  |                          |
| hydroxide           | Hf(OH) <sub>3</sub>                                                   | 25.40            | 4.0 × 10 <sup>-26</sup>  |
| Holmium             |                                                                       |                  |                          |
| hydroxide           | Ho(OH) <sub>3</sub>                                                   | 22.3             | 5.0 × 10 <sup>-23</sup>  |
| Indium              |                                                                       |                  |                          |
| ferrocyanide        | In <sub>4</sub> [Fe(CN) <sub>6</sub> ] <sub>3</sub>                   | 43.72            | 1.9 × 10 <sup>-44</sup>  |
| hydroxide           | In(OH) <sub>3</sub>                                                   | 33.2             | 6.3 × 10 <sup>-34</sup>  |
| quinolinolate       | InL <sub>3</sub>                                                      | 31.34            | 4.6 × 10 <sup>-32</sup>  |
| selenite            | In <sub>2</sub> (SeO <sub>3</sub> ) <sub>3</sub>                      | 32.60            | 4.0 × 10 <sup>-33</sup>  |
| sulfide             | In <sub>2</sub> S <sub>3</sub>                                        | 73.24            | 5.7 × 10 <sup>-74</sup>  |
| Iron(II)            |                                                                       |                  |                          |
| carbonate           | FeCO <sub>3</sub>                                                     | 10.50            | 3.13 × 10 <sup>-11</sup> |
| fluoride            | FeF <sub>2</sub>                                                      | 5.63             | 2.36 × 10 <sup>-6</sup>  |
| hydroxide           | Fe(OH) <sub>2</sub>                                                   | 16.31            | 4.87 × 10 <sup>-17</sup> |
| oxalate dihydrate   | FeC <sub>2</sub> O <sub>4</sub> · 2H <sub>2</sub> O                   | 6.50             | 3.2 × 10 <sup>-7</sup>   |
| sulfide             | FeS                                                                   | 17.20            | 6.3 × 10 <sup>-18</sup>  |
| Iron(III)           |                                                                       |                  |                          |
| arsenate            | FeAsO <sub>4</sub>                                                    | 20.24            | 5.7 × 10 <sup>-21</sup>  |
| ferrocyanide        | Fe <sub>4</sub> [Fe(CN) <sub>6</sub> ] <sub>3</sub>                   | 40.52            | 3.3 × 10 <sup>-41</sup>  |
| hydroxide           | Fe(OH) <sub>3</sub>                                                   | 38.55            | 2.79 × 10 <sup>-39</sup> |
| phosphate dihydrate | FePO <sub>4</sub> · 2H <sub>2</sub> O                                 | 15.00            | 9.91 × 10 <sup>-16</sup> |
| quinaldate          | FeL <sub>3</sub>                                                      | 16.89            | 1.3 × 10 <sup>-17</sup>  |
| selenite            | Fe <sub>2</sub> (SeO <sub>3</sub> ) <sub>3</sub>                      | 30.70            | 2.0 × 10 <sup>-31</sup>  |
| Lanthanum           |                                                                       |                  |                          |
| bromate 9-water     | La(BrO <sub>3</sub> ) <sub>3</sub> · 9H <sub>2</sub> O                | 2.50             | 3.2 × 10 <sup>-3</sup>   |
| fluoride            | LaF <sub>3</sub>                                                      | 16.2             | 7 × 10 <sup>-17</sup>    |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound             | Formula                                                | $pK_{sp}$ | $K_{sp}$               |
|----------------------|--------------------------------------------------------|-----------|------------------------|
| hydroxide            | $\text{La}(\text{OH})_3$                               | 18.70     | $2.0 \times 10^{-19}$  |
| iodate               | $\text{La}(\text{IO}_3)_3$                             | 11.12     | $7.50 \times 10^{-12}$ |
| molybdate            | $\text{La}_2(\text{MoO}_4)_3$                          | 20.4      | $4 \times 10^{-21}$    |
| oxalate 9-water      | $\text{La}_2(\text{C}_2\text{O}_4)_3$                  | 26.60     | $2.5 \times 10^{-27}$  |
| phosphate            | $\text{LaPO}_4$                                        | 22.43     | $3.7 \times 10^{-23}$  |
| sulfide              | $\text{La}_2\text{S}_3$                                | 12.70     | $2.0 \times 10^{-13}$  |
| tungstate trihydrate | $\text{La}_2(\text{WO}_4)_3 \cdot 3\text{H}_2\text{O}$ | 3.90      | $1.3 \times 10^{-4}$   |
| Lead                 |                                                        |           |                        |
| acetate              | $\text{Pb}(\text{OAc})_2$                              | 2.75      | $1.8 \times 10^{-3}$   |
| anthranilate         | $\text{PbL}_2$                                         | 9.81      | $1.6 \times 10^{-10}$  |
| arsenate             | $\text{Pb}_3(\text{AsO}_4)_3$                          | 35.39     | $4.0 \times 10^{-36}$  |
| azide                | $\text{Pb}(\text{N}_3)_2$                              | 8.59      | $2.5 \times 10^{-9}$   |
| borate, <i>meta</i>  | $\text{Pb}(\text{BO}_2)_3$                             | 10.78     | $1.6 \times 10^{-11}$  |
| bromate              | $\text{Pb}(\text{BrO}_3)_2$                            | 1.70      | $2.0 \times 10^{-2}$   |
| bromide              | $\text{PbBr}_2$                                        | 6.82      | $6.60 \times 10^{-6}$  |
| carbonate            | $\text{PbCO}_3$                                        | 13.13     | $7.4 \times 10^{-14}$  |
| chloride             | $\text{PbCl}_2$                                        | 4.77      | $1.70 \times 10^{-5}$  |
| chloride fluoride    | $\text{PbClF}$                                         | 8.62      | $2.4 \times 10^{-9}$   |
| chlorite             | $\text{Pb}(\text{ClO}_2)_2$                            | 8.4       | $4 \times 10^{-9}$     |
| chromate             | $\text{PbCrO}_4$                                       | 12.55     | $2.8 \times 10^{-13}$  |
| ferrocyanide         | $\text{Pb}_2[\text{Fe}(\text{CN})_6]$                  | 14.46     | $3.5 \times 10^{-15}$  |
| fluoride             | $\text{PbF}_2$                                         | 7.48      | $3.3 \times 10^{-8}$   |
| fluoride iodide      | $\text{PbFI}$                                          | 8.07      | $8.5 \times 10^{-9}$   |
| hydrogen phosphate   | $\text{PbHPO}_4$                                       | 9.90      | $1.3 \times 10^{-10}$  |
| hydrogen phosphite   | $\text{PbHPO}_3$                                       | 6.24      | $5.8 \times 10^{-7}$   |
| hydroxide            | $\text{Pb}(\text{OH})_2$                               | 14.84     | $1.43 \times 10^{-15}$ |
| hydroxide bromide    | $\text{PbOHBr}$                                        | 14.70     | $2.0 \times 10^{-15}$  |
| hydroxide chloride   | $\text{PbOHCl}$                                        | 13.7      | $2 \times 10^{-14}$    |
| hydroxide nitrate    | $\text{PbOHNO}_3$                                      | 3.55      | $2.8 \times 10^{-4}$   |
| iodate               | $\text{Pb}(\text{IO}_3)_2$                             | 12.43     | $3.69 \times 10^{-13}$ |
| iodide               | $\text{PbI}_2$                                         | 8.01      | $9.8 \times 10^{-9}$   |
| molybdate            | $\text{PbMoO}_4$                                       | 13.00     | $1.0 \times 10^{-13}$  |
| niobate              | $\text{Pb}(\text{NbO}_3)_2$                            | 16.62     | $2.4 \times 10^{-17}$  |
| oxalate              | $\text{PbC}_2\text{O}_4$                               | 9.32      | $4.8 \times 10^{-10}$  |
| phosphate            | $\text{Pb}_3(\text{PO}_4)_2$                           | 42.10     | $8.0 \times 10^{-43}$  |
| quinaldate           | $\text{PbL}_2$                                         | 10.60     | $2.5 \times 10^{-11}$  |
| selenate             | $\text{PbSeO}_4$                                       | 6.84      | $1.37 \times 10^{-7}$  |
| selenite             | $\text{PbSeO}_3$                                       | 11.50     | $3.2 \times 10^{-12}$  |
| sulfate              | $\text{PbSO}_4$                                        | 7.60      | $2.53 \times 10^{-8}$  |
| sulfide              | $\text{PbS}$                                           | 27.10     | $8.0 \times 10^{-28}$  |
| thiocyanate          | $\text{Pb}(\text{SCN})_2$                              | 4.70      | $2.0 \times 10^{-5}$   |
| thiosulfate          | $\text{PbS}_2\text{O}_3$                               | 6.40      | $4.0 \times 10^{-7}$   |
| tungstate            | $\text{PbWO}_4$                                        | 6.35      | $4.5 \times 10^{-7}$   |
| Lead(IV)             |                                                        |           |                        |
| hydroxide            | $\text{Pb}(\text{OH})_4$                               | 65.50     | $3.2 \times 10^{-66}$  |
| Lithium              |                                                        |           |                        |
| carbonate            | $\text{Li}_2\text{CO}_3$                               | 1.60      | $2.5 \times 10^{-2}$   |
| fluoride             | $\text{LiF}$                                           | 2.74      | $1.84 \times 10^{-3}$  |
| phosphate            | $\text{Li}_3\text{PO}_4$                               | 10.63     | $2.37 \times 10^{-11}$ |
| uranylarsenate       | $\text{LiUO}_2\text{AsO}_4$                            | 18.82     | $1.5 \times 10^{-19}$  |
| Lutetium             |                                                        |           |                        |
| hydroxide            | $\text{Lu}(\text{OH})_3$                               | 23.72     | $1.9 \times 10^{-24}$  |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound             | Formula                                                             | pK <sub>sp</sub> | K <sub>sp</sub>        |
|----------------------|---------------------------------------------------------------------|------------------|------------------------|
| <b>Magnesium</b>     |                                                                     |                  |                        |
| ammonium phosphate   | MgNH <sub>4</sub> PO <sub>4</sub>                                   | 12.60            | $2.5 \times 10^{-13}$  |
| arsenate             | Mg <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>                    | 19.68            | $2.1 \times 10^{-20}$  |
| carbonate            | MgCO <sub>3</sub>                                                   | 5.17             | $6.82 \times 10^{-6}$  |
| carbonate trihydrate | MgCO <sub>3</sub> · 3H <sub>2</sub> O                               | 5.62             | $2.38 \times 10^{-6}$  |
| fluoride             | MgF <sub>2</sub>                                                    | 10.29            | $5.16 \times 10^{-11}$ |
| hydroxide            | Mg(OH) <sub>2</sub>                                                 | 11.25            | $5.61 \times 10^{-12}$ |
| iodate 4-water       | Mg(IO <sub>3</sub> ) <sub>2</sub> · 4H <sub>2</sub> O               | 2.50             | $3.2 \times 10^{-3}$   |
| niobate              | Mg(NbO <sub>3</sub> ) <sub>2</sub>                                  | 16.64            | $2.3 \times 10^{-17}$  |
| oxalate dihydrate    | MgC <sub>2</sub> O <sub>4</sub> · 2H <sub>2</sub> O                 | 5.32             | $4.83 \times 10^{-6}$  |
| phosphate            | Mg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>                     | 23.98            | $1.04 \times 10^{-24}$ |
| 8-quinolinolate      | MgL <sub>2</sub>                                                    | 15.40            | $4.0 \times 10^{-16}$  |
| selenite             | MgSeO <sub>3</sub>                                                  | 4.89             | $1.3 \times 10^{-5}$   |
| sulfite              | MgSO <sub>3</sub>                                                   | 2.50             | $3.2 \times 10^{-3}$   |
| <b>Manganese</b>     |                                                                     |                  |                        |
| anthranilate         | MnL <sub>2</sub>                                                    | 6.75             | $1.8 \times 10^{-3}$   |
| arsenate             | Mn <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>                    | 28.72            | $1.9 \times 10^{-29}$  |
| carbonate            | MnCO <sub>3</sub>                                                   | 10.63            | $2.34 \times 10^{-11}$ |
| ferrocyanide         | Mn <sub>2</sub> [Fe(CN) <sub>6</sub> ]                              | 12.10            | $8.0 \times 10^{-13}$  |
| iodate               | Mn(IO <sub>3</sub> ) <sub>2</sub>                                   | 6.36             | $4.37 \times 10^{-7}$  |
| hydroxide            | Mn(OH) <sub>2</sub>                                                 | 12.72            | $1.9 \times 10^{-13}$  |
| oxalate dihydrate    | MnC <sub>2</sub> O <sub>4</sub> · 2H <sub>2</sub> O                 | 6.77             | $1.70 \times 10^{-7}$  |
| 8-quinolinolate      | MnL <sub>2</sub>                                                    | 21.70            | $2.0 \times 10^{-22}$  |
| selenite             | MnSeO <sub>3</sub>                                                  | 6.90             | $1.3 \times 10^{-7}$   |
| sulfide              | MnS amorphous                                                       | 9.60             | $2.5 \times 10^{-10}$  |
|                      | MnS crystalline                                                     | 12.60            | $2.5 \times 10^{-13}$  |
| <b>Mercury(I)</b>    |                                                                     |                  |                        |
| azide                | Hg <sub>2</sub> (N <sub>3</sub> ) <sub>2</sub>                      | 9.15             | $7.1 \times 10^{-10}$  |
| bromide              | Hg <sub>2</sub> Br <sub>2</sub>                                     | 22.19            | $6.40 \times 10^{-23}$ |
| carbonate            | Hg <sub>2</sub> CO <sub>3</sub>                                     | 16.44            | $3.6 \times 10^{-17}$  |
| chloride             | Hg <sub>2</sub> Cl <sub>2</sub>                                     | 17.84            | $1.43 \times 10^{-18}$ |
| cyanide              | Hg <sub>2</sub> (CN) <sub>2</sub>                                   | 39.3             | $5 \times 10^{-40}$    |
| chromate             | Hg <sub>2</sub> CrO <sub>4</sub>                                    | 8.70             | $2.0 \times 10^{-9}$   |
| ferricyanide         | (Hg <sub>2</sub> ) <sub>3</sub> [Fe(CN) <sub>6</sub> ] <sub>2</sub> | 20.07            | $8.5 \times 10^{-21}$  |
| fluoride             | Hg <sub>2</sub> F <sub>2</sub>                                      | 5.51             | $3.10 \times 10^{-6}$  |
| hydrogen phosphate   | Hg <sub>2</sub> HPO <sub>4</sub>                                    | 12.40            | $4.0 \times 10^{-13}$  |
| hydroxide            | Hg <sub>2</sub> (OH) <sub>2</sub>                                   | 23.70            | $2.0 \times 10^{-24}$  |
| iodate               | Hg <sub>2</sub> (IO <sub>3</sub> ) <sub>2</sub>                     | 13.71            | $2.0 \times 10^{-14}$  |
| iodide               | Hg <sub>2</sub> I <sub>2</sub>                                      | 28.72            | $5.2 \times 10^{-29}$  |
| oxalate              | Hg <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                       | 12.76            | $1.75 \times 10^{-13}$ |
| quinaldate           | Hg <sub>2</sub> L <sub>2</sub>                                      | 17.90            | $1.3 \times 10^{-18}$  |
| selenite             | Hg <sub>2</sub> SeO <sub>3</sub>                                    | 14.20            | $8.4 \times 10^{-15}$  |
| sulfate              | Hg <sub>2</sub> SO <sub>4</sub>                                     | 6.19             | $6.5 \times 10^{-7}$   |
| sulfite              | Hg <sub>2</sub> SO <sub>3</sub>                                     | 27.0             | $1.0 \times 10^{-27}$  |
| sulfide              | Hg <sub>2</sub> S                                                   | 47.0             | $1.0 \times 10^{-47}$  |
| thiocyanate          | Hg <sub>2</sub> (SCN) <sub>2</sub>                                  | 19.49            | $3.2 \times 10^{-20}$  |
| tungstate            | Hg <sub>2</sub> WO <sub>4</sub>                                     | 16.96            | $1.1 \times 10^{-17}$  |
| <b>Mercury(II)</b>   |                                                                     |                  |                        |
| bromide              | HgBr <sub>2</sub>                                                   | 19.21            | $6.2 \times 10^{-20}$  |
| hydroxide            | Hg(OH) <sub>2</sub>                                                 | 25.52            | $3.2 \times 10^{-26}$  |
| iodate               | Hg(IO <sub>3</sub> ) <sub>2</sub>                                   | 12.49            | $3.2 \times 10^{-13}$  |
| iodide               | HgI <sub>2</sub>                                                    | 28.54            | $2.9 \times 10^{-29}$  |
| 1,10-phenanthroline  | HgL <sub>2</sub>                                                    | 24.70            | $2.0 \times 10^{-25}$  |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound                | Formula                   | $pK_{sp}$ | $K_{sp}$               |
|-------------------------|---------------------------|-----------|------------------------|
| quinaldate              | $HgL_2$                   | 16.80     | $1.6 \times 10^{-17}$  |
| selenite                | $HgSeO_3$                 | 13.82     | $1.5 \times 10^{-14}$  |
| sulfide                 | $HgS$ red                 | 52.4      | $4 \times 10^{-53}$    |
|                         | $HgS$ black               | 51.80     | $1.6 \times 10^{-52}$  |
| Neodymium               |                           |           |                        |
| carbonate               | $Nd_2(CO_3)_3$            | 32.97     | $1.08 \times 10^{-33}$ |
| hydroxide               | $Nd(OH)_3$                | 21.49     | $3.2 \times 10^{-22}$  |
| Neptunyl(VI)            |                           |           |                        |
| hydroxide               | $NpO_2(OH)_2$             | 21.60     | $2.5 \times 10^{-22}$  |
| Nickel                  |                           |           |                        |
| ammine perrhenate       | $[Ni(NH_3)_6][ReO_4]_2$   | 3.29      | $5.1 \times 10^{-4}$   |
| anthranilate            | $NiL_2$                   | 9.09      | $8.1 \times 10^{-10}$  |
| arsenate                | $Ni_3(AsO_4)_2$           | 25.51     | $3.1 \times 10^{-26}$  |
| carbonate               | $NiCO_3$                  | 6.85      | $1.42 \times 10^{-7}$  |
| ferrocyanide            | $Ni_2[Fe(CN)_6]$          | 14.89     | $1.3 \times 10^{-15}$  |
| hydrazine sulfate       | $[Ni(N_2H_4)_3]SO_4$      | 13.15     | $7.1 \times 10^{-15}$  |
| hydroxide               | $Ni(OH)_2$ fresh          | 15.26     | $5.48 \times 10^{-16}$ |
| iodate                  | $Ni(IO_3)_2$              | 4.33      | $4.71 \times 10^{-5}$  |
| oxalate                 | $NiC_2O_4$                | 9.4       | $4 \times 10^{-10}$    |
| phosphate               | $Ni_3(PO_4)_2$            | 31.32     | $4.74 \times 10^{-32}$ |
| pyrophosphate           | $Ni_2P_2O_7$              | 12.77     | $1.7 \times 10^{-13}$  |
| quinaldate              | $NiL_2$                   | 10.1      | $8 \times 10^{-11}$    |
| 8-quinolinolate         | $NiL_2$                   | 26.1      | $8 \times 10^{-27}$    |
| selenite                | $NiSeO_3$                 | 5.0       | $1.0 \times 10^{-5}$   |
| $\alpha$ -sulfide       | $\alpha$ -NiS             | 18.50     | $3.2 \times 10^{-19}$  |
| $\beta$ -sulfide        | $\beta$ -NiS              | 24.0      | $1.0 \times 10^{-24}$  |
| $\gamma$ -sulfide       | $\gamma$ -NiS             | 25.70     | $2.0 \times 10^{-26}$  |
| Palladium               |                           |           |                        |
| (II) hydroxide          | $Pd(OH)_2$                | 31.0      | $1.0 \times 10^{-31}$  |
| (IV) hydroxide          | $Pd(OH)_4$                | 70.20     | $6.3 \times 10^{-71}$  |
| quinaldate              | $PdL_2$                   | 12.90     | $1.3 \times 10^{-13}$  |
| thiocyanate             | $Pd(SCN)_2$               | 22.36     | $4.39 \times 10^{-23}$ |
| Platinum                |                           |           |                        |
| (IV) bromide            | $PtBr_4$                  | 40.50     | $3.2 \times 10^{-41}$  |
| (II) hydroxide          | $Pt(OH)_2$                | 35        | $1 \times 10^{-35}$    |
| Plutonium               |                           |           |                        |
| (III) fluoride          | $PuF_3$                   | 15.60     | $2.5 \times 10^{-16}$  |
| (IV) fluoride           | $PuF_4$                   | 19.20     | $6.3 \times 10^{-20}$  |
| (IV) hydrogen phosphate | $Pu(HPO_4)_2 \cdot xH_2O$ | 27.7      | $2 \times 10^{-28}$    |
| (III) hydroxide         | $Pu(OH)_3$                | 19.70     | $2.0 \times 10^{-20}$  |
| (IV) hydroxide          | $Pu(OH)_4$                | 55        | $1 \times 10^{-55}$    |
| (IV) iodate             | $Pu(IO_3)_4$              | 12.3      | $5 \times 10^{-13}$    |
| (VI) carbonate          | $PuO_2CO_3$               | 12.77     | $1.7 \times 10^{-13}$  |
| (V) hydroxide           | $PuO_2(OH)$               | 9.3       | $5 \times 10^{-10}$    |
| (VI) hydroxide          | $PuO_2(OH)_2$             | 24.7      | $2 \times 10^{-25}$    |
| Polonium                |                           |           |                        |
| sulfide                 | $PoS$                     | 28.26     | $5.6 \times 10^{-29}$  |
| Potassium               |                           |           |                        |
| hexabromoplatinate      | $K_2[PtBr_6]$             | 4.20      | $6.3 \times 10^{-5}$   |
| hexachloropalladate     | $K_2[PdCl_6]$             | 5.22      | $6.0 \times 10^{-6}$   |
| hexachloroplatinate     | $K_2[PtCl_6]$             | 5.13      | $7.48 \times 10^{-6}$  |
| hexafluoroplatinate     | $K_2[PtF_6]$              | 4.54      | $2.9 \times 10^{-5}$   |

TABLE 8.6 Solubility Product Constants (Continued)

| Compound                      | Formula                                                                  | pK <sub>sp</sub> | K <sub>sp</sub>          |
|-------------------------------|--------------------------------------------------------------------------|------------------|--------------------------|
| hexafluorosilicate            | K <sub>2</sub> [SiF <sub>6</sub> ]                                       | 6.06             | 8.7 × 10 <sup>-7</sup>   |
| hexafluorozirconate           | K <sub>2</sub> [ZrF <sub>6</sub> ]                                       | 3.3              | 5 × 10 <sup>-4</sup>     |
| iodate                        | KIO <sub>4</sub>                                                         | 3.43             | 3.74 × 10 <sup>-4</sup>  |
| perchlorate                   | KClO <sub>4</sub>                                                        | 1.98             | 1.05 × 10 <sup>-2</sup>  |
| sodium cobaltinitrite hydrate | K <sub>2</sub> Na[Co(NO <sub>2</sub> ) <sub>6</sub> ] · H <sub>2</sub> O | 10.66            | 2.2 × 10 <sup>-11</sup>  |
| tetraphenylborate             | K[B(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> ]                       | 7.66             | 2.2 × 10 <sup>-8</sup>   |
| uranyl arsenate               | K[UO <sub>2</sub> AsO <sub>4</sub> ]                                     | 22.60            | 2.5 × 10 <sup>-23</sup>  |
| uranyl carbonate              | K <sub>4</sub> [UO <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub> ]        | 4.20             | 6.3 × 10 <sup>-5</sup>   |
| Praseodymium hydroxide        | Pr(OH) <sub>3</sub>                                                      | 23.45            | 3.39 × 10 <sup>-24</sup> |
| Promethium hydroxide          | Pm(OH) <sub>3</sub>                                                      | 21               | 1 × 10 <sup>-21</sup>    |
| Radium iodate                 | Ra(IO <sub>3</sub> ) <sub>2</sub>                                        | 8.94             | 1.16 × 10 <sup>-9</sup>  |
| Radium sulfate                | RaSO <sub>4</sub>                                                        | 10.44            | 3.66 × 10 <sup>-11</sup> |
| Rhodium hydroxide             | Rh(OH) <sub>3</sub>                                                      | 23               | 1 × 10 <sup>-23</sup>    |
| Rubidium cobaltinitrite       | Rb <sub>3</sub> [Co(NO <sub>2</sub> ) <sub>6</sub> ]                     | 14.83            | 1.5 × 10 <sup>-15</sup>  |
| hexachloroplatinate           | Rb <sub>2</sub> [PtCl <sub>6</sub> ]                                     | 7.20             | 6.3 × 10 <sup>-8</sup>   |
| hexafluoroplatinate           | Rb <sub>2</sub> [PtF <sub>6</sub> ]                                      | 6.12             | 7.7 × 10 <sup>-7</sup>   |
| hexafluorosilicate            | Rb <sub>2</sub> [SiF <sub>6</sub> ]                                      | 6.30             | 5.0 × 10 <sup>-7</sup>   |
| perchlorate                   | RbClO <sub>4</sub>                                                       | 2.52             | 3.0 × 10 <sup>-3</sup>   |
| periodate                     | RbIO <sub>4</sub>                                                        | 3.26             | 5.5 × 10 <sup>-4</sup>   |
| Ruthenium hydroxide           | Ru(OH) <sub>3</sub>                                                      | 36               | 1 × 10 <sup>-36</sup>    |
| Samarium hydroxide            | Sm(OH) <sub>3</sub>                                                      | 22.08            | 8.3 × 10 <sup>-23</sup>  |
| Scandium fluoride             | ScF <sub>3</sub>                                                         | 23.24            | 5.81 × 10 <sup>-24</sup> |
| Scandium hydroxide            | Sc(OH) <sub>3</sub>                                                      | 30.65            | 2.22 × 10 <sup>-31</sup> |
| Silver acetate                | AgOAc                                                                    | 2.71             | 1.94 × 10 <sup>-3</sup>  |
| arsenate                      | Ag <sub>3</sub> AsO <sub>4</sub>                                         | 21.99            | 1.03 × 10 <sup>-22</sup> |
| azide                         | AgN <sub>3</sub>                                                         | 8.54             | 2.8 × 10 <sup>-9</sup>   |
| bromate                       | AgBrO <sub>3</sub>                                                       | 4.27             | 5.38 × 10 <sup>-5</sup>  |
| bromide                       | AgBr                                                                     | 12.27            | 5.35 × 10 <sup>-13</sup> |
| carbonate                     | Ag <sub>2</sub> CO <sub>3</sub>                                          | 11.07            | 8.46 × 10 <sup>-12</sup> |
| chloride                      | AgCl                                                                     | 9.75             | 1.77 × 10 <sup>-10</sup> |
| chlorite                      | AgClO <sub>2</sub>                                                       | 3.70             | 2.0 × 10 <sup>-4</sup>   |
| chromate                      | Ag <sub>2</sub> CrO <sub>4</sub>                                         | 11.95            | 1.12 × 10 <sup>-12</sup> |
| cobaltinitrite                | Ag <sub>3</sub> [Co(NO <sub>2</sub> ) <sub>6</sub> ]                     | 20.07            | 8.5 × 10 <sup>-21</sup>  |
| cyanamide                     | Ag <sub>2</sub> CN <sub>2</sub>                                          | 10.14            | 7.2 × 10 <sup>-11</sup>  |
| cyanate                       | AgOCN                                                                    | 6.64             | 2.3 × 10 <sup>-7</sup>   |
| cyanide                       | AgCN                                                                     | 16.22            | 5.97 × 10 <sup>-17</sup> |
| dichromate                    | Ag <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>                           | 6.70             | 2.0 × 10 <sup>-7</sup>   |
| dicyanamide                   | AgN(CN) <sub>2</sub>                                                     | 8.85             | 1.4 × 10 <sup>-9</sup>   |
| ferrocyanide                  | Ag <sub>4</sub> [Fe(CN) <sub>6</sub> ]                                   | 40.81            | 1.6 × 10 <sup>-41</sup>  |
| hydroxide                     | AgOH                                                                     | 7.71             | 2.0 × 10 <sup>-8</sup>   |
| hyponitrite                   | Ag <sub>2</sub> N <sub>2</sub> O <sub>2</sub>                            | 18.89            | 1.3 × 10 <sup>-19</sup>  |
| iodate                        | AgIO <sub>3</sub>                                                        | 7.50             | 3.17 × 10 <sup>-8</sup>  |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound                | Formula                          | $pK_{sp}$ | $K_{sp}$               |
|-------------------------|----------------------------------|-----------|------------------------|
| iodide                  | AgI                              | 16.07     | $8.52 \times 10^{-17}$ |
| molybdate               | $Ag_2MoO_4$                      | 11.55     | $2.8 \times 10^{-12}$  |
| nitrite                 | AgNO <sub>2</sub>                | 3.22      | $6.0 \times 10^{-4}$   |
| oxalate                 | $Ag_2C_2O_4$                     | 11.27     | $5.40 \times 10^{-12}$ |
| phosphate               | $Ag_3PO_4$                       | 16.05     | $8.89 \times 10^{-17}$ |
| quinaldate              | AgL                              | 16.89     | $1.3 \times 10^{-17}$  |
| perrhenate              | AgReO <sub>4</sub>               | 4.10      | $8.0 \times 10^{-5}$   |
| selenate                | $Ag_2SeO_4$                      | 7.25      | $5.7 \times 10^{-8}$   |
| selenite                | $Ag_2SeO_3$                      | 15.00     | $1.0 \times 10^{-15}$  |
| selenocyanate           | AgSeCN                           | 15.40     | $4.0 \times 10^{-16}$  |
| sulfate                 | $Ag_2SO_4$                       | 4.92      | $1.20 \times 10^{-5}$  |
| sulfite                 | $Ag_2SO_3$                       | 13.82     | $1.50 \times 10^{-14}$ |
| sulfide                 | $Ag_2S$                          | 49.20     | $6.3 \times 10^{-50}$  |
| thiocyanate             | AgSCN                            | 11.99     | $1.03 \times 10^{-12}$ |
| vanadate                | AgVO <sub>3</sub>                | 6.3       | $5 \times 10^{-7}$     |
| tungstate               | $Ag_2WO_4$                       | 11.26     | $5.5 \times 10^{-12}$  |
| Sodium                  |                                  |           |                        |
| ammonium cobaltinitrite | $Na(NH_4)_2[Co(NO_2)_6]$         | 10.66     | $2.2 \times 10^{-11}$  |
| antimonate              | $Na[Sb(OH)_6]$                   | 7.4       | $4 \times 10^{-8}$     |
| hexafluoroaluminate     | $Na_2[AlF_6]$                    | 9.39      | $4.0 \times 10^{-10}$  |
| uranyl arsenate         | $NaUO_2AsO_4$                    | 21.87     | $1.3 \times 10^{-22}$  |
| Strontium               |                                  |           |                        |
| arsenate                | $Sr_3(AsO_4)_2$                  | 18.37     | $4.29 \times 10^{-19}$ |
| carbonate               | SrCO <sub>3</sub>                | 9.25      | $5.60 \times 10^{-10}$ |
| chromate                | SrCrO <sub>4</sub>               | 4.65      | $2.2 \times 10^{-5}$   |
| fluoride                | SrF <sub>2</sub>                 | 8.36      | $4.33 \times 10^{-9}$  |
| iodate                  | $Sr(IO_3)_2$                     | 6.94      | $1.14 \times 10^{-7}$  |
| iodate hydrate          | $Sr(IO_3)_2 \cdot H_2O$          | 6.42      | $3.77 \times 10^{-7}$  |
| molybdate               | SrMoO <sub>4</sub>               | 6.7       | $2 \times 10^{-7}$     |
| niobate                 | $Sr(NbO_3)_2$                    | 17.38     | $4.2 \times 10^{-18}$  |
| oxalate hydrate         | $SrC_2O_4 \cdot H_2O$            | 6.80      | $1.6 \times 10^{-7}$   |
| phosphate               | $Sr_3(PO_4)_2$                   | 27.39     | $4.0 \times 10^{-28}$  |
| 8-quinolinolate         | SrL <sub>2</sub>                 | 9.3       | $5 \times 10^{-10}$    |
| selenate                | SrSeO <sub>4</sub>               | 3.09      | $8.1 \times 10^{-4}$   |
| selenite                | SrSeO <sub>3</sub>               | 5.74      | $1.8 \times 10^{-6}$   |
| sulfate                 | SrSO <sub>4</sub>                | 6.46      | $3.44 \times 10^{-7}$  |
| sulfite                 | SrSO <sub>3</sub>                | 7.4       | $4 \times 10^{-8}$     |
| tungstate               | SrWO <sub>4</sub>                | 9.77      | $1.7 \times 10^{-10}$  |
| Terbium                 |                                  |           |                        |
| hydroxide               | Tb(OH) <sub>3</sub>              | 21.70     | $2.0 \times 10^{-22}$  |
| Tellurium               |                                  |           |                        |
| hydroxide               | Te(OH) <sub>4</sub>              | 53.52     | $3.0 \times 10^{-54}$  |
| Thallium(I)             |                                  |           |                        |
| azide                   | TlN <sub>3</sub>                 | 3.66      | $2.2 \times 10^{-4}$   |
| bromate                 | TlBrO <sub>3</sub>               | 4.96      | $1.10 \times 10^{-5}$  |
| bromide                 | TlBr                             | 5.43      | $3.71 \times 10^{-6}$  |
| chloride                | TlCl                             | 3.73      | $1.86 \times 10^{-4}$  |
| chromate                | Tl <sub>2</sub> CrO <sub>4</sub> | 12.06     | $8.67 \times 10^{-13}$ |
| ferrocyanide dihydrate  | $Tl_4[Fe(CN)_6] \cdot 2H_2O$     | 9.3       | $5 \times 10^{-10}$    |
| hexachloroplatinate     | $Tl_2[PtCl_6]$                   | 11.40     | $4.0 \times 10^{-12}$  |
| iodate                  | TlIO <sub>3</sub>                | 5.51      | $3.12 \times 10^{-6}$  |
| iodide                  | TlI                              | 7.26      | $5.54 \times 10^{-8}$  |



TABLE 8.6 Solubility Product Constants (Continued)

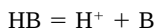
| Compound             | Formula                                                           | pK <sub>sp</sub> | K <sub>sp</sub>          |
|----------------------|-------------------------------------------------------------------|------------------|--------------------------|
| oxalate              | Tl <sub>2</sub> C <sub>2</sub> O <sub>4</sub>                     | 3.7              | 2 × 10 <sup>-4</sup>     |
| selenate             | Tl <sub>2</sub> SeO <sub>4</sub>                                  | 4.00             | 1.0 × 10 <sup>-4</sup>   |
| selenite             | Tl <sub>2</sub> SeO <sub>3</sub>                                  | 38.7             | 2 × 10 <sup>-39</sup>    |
| sulfide              | Tl <sub>2</sub> S                                                 | 20.30            | 5.0 × 10 <sup>-21</sup>  |
| thiocyanate          | TlSCN                                                             | 3.80             | 1.57 × 10 <sup>-4</sup>  |
| Thallium(III)        |                                                                   |                  |                          |
| hydroxide            | Tl(OH) <sub>3</sub>                                               | 43.77            | 1.68 × 10 <sup>-44</sup> |
| 8-quinolinolate      | TlL <sub>3</sub>                                                  | 32.40            | 4.0 × 10 <sup>-33</sup>  |
| Thorium              |                                                                   |                  |                          |
| hydrogen phosphate   | Th(HPO <sub>4</sub> ) <sub>2</sub>                                | 20               | 1 × 10 <sup>-20</sup>    |
| hydroxide            | Th(OH) <sub>4</sub>                                               | 44.40            | 4.0 × 10 <sup>-45</sup>  |
| iodate               | Th(IO <sub>3</sub> ) <sub>4</sub>                                 | 14.60            | 2.5 × 10 <sup>-15</sup>  |
| oxalate              | Th(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub>                   | 22               | 1 × 10 <sup>-22</sup>    |
| phosphate            | Th <sub>3</sub> (PO <sub>4</sub> ) <sub>4</sub>                   | 78.60            | 2.5 × 10 <sup>-79</sup>  |
| Thulium              |                                                                   |                  |                          |
| hydroxide            | Tm(OH) <sub>3</sub>                                               | 23.48            | 3.3 × 10 <sup>-24</sup>  |
| Tin                  |                                                                   |                  |                          |
| (II) hydroxide       | Sn(OH) <sub>2</sub>                                               | 27.26            | 5.45 × 10 <sup>-28</sup> |
| (IV) hydroxide       | Sn(OH) <sub>4</sub>                                               | 56               | 1 × 10 <sup>-56</sup>    |
| (II) sulfide         | SnS                                                               | 25.00            | 1.0 × 10 <sup>-25</sup>  |
| Titanium             |                                                                   |                  |                          |
| (III) hydroxide      | Ti(OH) <sub>3</sub>                                               | 40               | 1 × 10 <sup>-40</sup>    |
| (IV) oxide hydroxide | TiO(OH) <sub>2</sub>                                              | 29               | 1 × 10 <sup>-29</sup>    |
| Uranium(IV)          |                                                                   |                  |                          |
| fluoride 2.5-water   | UF <sub>4</sub> ·2.5H <sub>2</sub> O                              | 21.24            | 5.7 × 10 <sup>-22</sup>  |
| Uranyl(VI)(2+)       |                                                                   |                  |                          |
| carbonate            | UO <sub>2</sub> CO <sub>3</sub>                                   | 11.73            | 1.8 × 10 <sup>-12</sup>  |
| ferrocyanide         | UO <sub>2</sub> [Fe(CN) <sub>6</sub> ]                            | 13.15            | 7.1 × 10 <sup>-14</sup>  |
| hydrogen arsenate    | UO <sub>2</sub> HAsO <sub>4</sub>                                 | 10.50            | 3.2 × 10 <sup>-11</sup>  |
| hydrogen phosphate   | UO <sub>2</sub> HPO <sub>4</sub>                                  | 10.67            | 2.1 × 10 <sup>-11</sup>  |
| hydroxide            | UO <sub>2</sub> (OH) <sub>2</sub>                                 | 21.95            | 1.1 × 10 <sup>-22</sup>  |
| iodate hydrate       | UO <sub>2</sub> (IO <sub>3</sub> ) <sub>2</sub> ·H <sub>2</sub> O | 7.50             | 3.2 × 10 <sup>-8</sup>   |
| oxalate trihydrate   | UO <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·3H <sub>2</sub> O  | 3.7              | 2 × 10 <sup>-4</sup>     |
| phosphate            | (UO <sub>2</sub> ) <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>   | 46.7             | 2 × 10 <sup>-47</sup>    |
| sulfite              | UO <sub>2</sub> SO <sub>3</sub>                                   | 8.58             | 2.6 × 10 <sup>-9</sup>   |
| thiocyanate          | (UO <sub>2</sub> )(SCN) <sub>2</sub>                              | 3.4              | 4 × 10 <sup>-4</sup>     |
| Vanadium             |                                                                   |                  |                          |
| (IV) hydroxide       | VO(OH) <sub>2</sub>                                               | 22.13            | 5.9 × 10 <sup>-23</sup>  |
| (III) phosphate      | (VO <sub>2</sub> ) <sub>3</sub> PO <sub>4</sub>                   | 24.1             | 8 × 10 <sup>-25</sup>    |
| Ytterbium            |                                                                   |                  |                          |
| hydroxide            | Yt(OH) <sub>3</sub>                                               | 23.60            | 2.5 × 10 <sup>-24</sup>  |
| Yttrium              |                                                                   |                  |                          |
| carbonate            | Y <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub>                    | 2.99             | 1.03 × 10 <sup>-3</sup>  |
| fluoride             | YF <sub>3</sub>                                                   | 20.06            | 8.62 × 10 <sup>-21</sup> |
| hydroxide            | Y(OH) <sub>3</sub>                                                | 22.00            | 1.00 × 10 <sup>-22</sup> |
| iodate               | Y(IO <sub>3</sub> ) <sub>3</sub>                                  | 9.95             | 1.12 × 10 <sup>-10</sup> |
| oxalate              | Y <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>      | 28.28            | 5.3 × 10 <sup>-29</sup>  |
| Zinc                 |                                                                   |                  |                          |
| anthranilate         | ZnL <sub>2</sub>                                                  | 9.23             | 5.9 × 10 <sup>-10</sup>  |
| arsenate             | Zn <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>                  | 27.55            | 2.8 × 10 <sup>-28</sup>  |
| borate hydrate       | Zn(BO <sub>2</sub> ) <sub>2</sub> ·H <sub>2</sub> O               | 10.18            | 6.6 × 10 <sup>-11</sup>  |
| carbonate            | ZnCO <sub>3</sub>                                                 | 9.94             | 1.46 × 10 <sup>-10</sup> |
| ferrocyanide         | Zn <sub>2</sub> [Fe(CN) <sub>6</sub> ]                            | 15.40            | 4.0 × 10 <sup>-15</sup>  |

**TABLE 8.6** Solubility Product Constants (*Continued*)

| Compound          | Formula                  | $pK_{sp}$ | $K_{sp}$              |
|-------------------|--------------------------|-----------|-----------------------|
| fluoride          | $ZnF_2$                  | 1.52      | $3.04 \times 10^{-2}$ |
| hydroxide         | $Zn(OH)_2$               | 16.5      | $3 \times 10^{-17}$   |
| iodate dihydrate  | $Zn(IO_3)_2 \cdot 2H_2O$ | 5.37      | $4.1 \times 10^{-6}$  |
| oxalate dihydrate | $ZnC_2O_4 \cdot 2H_2O$   | 8.86      | $1.38 \times 10^{-9}$ |
| phosphate         | $Zn_3(PO_4)_2$           | 32.04     | $9.0 \times 10^{-33}$ |
| quinaldate        | $ZnL_2$                  | 13.80     | $1.6 \times 10^{-14}$ |
| 8-quinolinolate   | $ZnL_2$                  | 24.30     | $5.0 \times 10^{-25}$ |
| selenide          | $ZnSe$                   | 25.44     | $3.6 \times 10^{-26}$ |
| selenite hydrate  | $ZnSeO_3 \cdot H_2O$     | 6.80      | $1.57 \times 10^{-7}$ |
| sulfide           | $\alpha\text{-ZnS}$      | 23.80     | $1.6 \times 10^{-24}$ |
|                   | $\beta\text{-ZnS}$       | 21.60     | $2.5 \times 10^{-22}$ |
| Zirconium         |                          |           |                       |
| oxide hydroxide   | $ZrO(OH)_2$              | 48.20     | $6.3 \times 10^{-49}$ |
| phosphate         | $Zr_3(PO_4)_4$           | 132       | $1 \times 10^{-132}$  |

### 8.2.1 Proton-Transfer Reactions

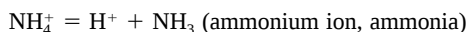
The  $pK_a$  values listed in Tables 8.7 and 8.8 are the negative (decadic) logarithms of the acidic dissociation constant, i.e.,  $-\log_{10} K_a = pK_a$ . For the general proton-transfer reaction



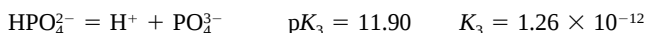
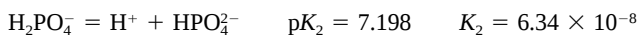
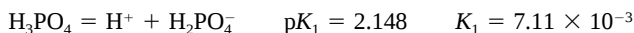
the acidic dissociation constant is formulated as follows:

$$K_a = \frac{[H^+][B]}{[HB]}$$

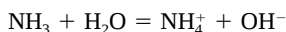
The most common charge types for the acid HB and its conjugate base B are



Acids which have more than one acidic hydrogen ionize in steps, as shown for phosphoric acid:



If the basic dissociation constant  $K_b$  for the equilibrium such as



is required,  $pK_b$  may be calculated from the relationship

$$pK_b = pK_w - pK_a$$

**TABLE 8.7** Proton Transfer Reactions of Inorganic Materials in Water at 25°C

| Substance                       | Formula or remarks                                                                     | p <i>K</i> <sub>1</sub>      | p <i>K</i> <sub>2</sub> |
|---------------------------------|----------------------------------------------------------------------------------------|------------------------------|-------------------------|
| Aluminic acid                   | H <sub>3</sub> AlO <sub>3</sub>                                                        | 11.2                         |                         |
| Aluminum ion (aquo)             | Al <sup>3+</sup> (aquo)                                                                | 4.98(4)                      |                         |
| Americium(III) ion              | Am <sup>3+</sup> (aquo) $\mu$ = 0.1                                                    | 5.92                         |                         |
| Ammonium ion                    | NH <sub>4</sub> <sup>+</sup>                                                           | 9.246(2)                     |                         |
| Ammonium- <i>d</i> <sub>3</sub> | ND <sub>3</sub> H <sup>+</sup>                                                         | 9.757                        |                         |
| Antimonic acid                  | HSb(OH) <sub>6</sub> = Sb(OH) <sub>6</sub> <sup>−</sup> + H <sup>+</sup> $\mu$ = 0.5   | 2.55                         |                         |
| Antimony(III) ion               | SbO <sup>+</sup> + H <sub>2</sub> O = Sb(OH) <sub>3</sub> + H <sup>+</sup> $\mu$ = 1.0 | 1.42                         |                         |
| Barium ion                      | p <i>K</i> <sub>b</sub> of Ba(OH) <sup>+</sup> $\mu$ = 0.1                             | 0.64                         |                         |
| Berkelium(III) ion              | p <i>K</i> for hydrolysis of Bk <sup>3+</sup> $\mu$ = 0.1                              | 5.66                         |                         |
| Beryllium(II) ion               | Be <sup>2+</sup> (aquo) = BeOH <sup>+</sup> + H <sup>+</sup> $\mu$ = 1.0               | 6.5                          |                         |
| Bismuth(III) ion                | Bi <sup>3+</sup> = BiOH <sup>2+</sup> + H <sup>+</sup> $\mu$ = 3.0                     | 1.58                         |                         |
| Boric acid, tetra-              | H <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                                           | 4                            | 9                       |
| Bromine                         | Br <sub>2</sub> + H <sub>2</sub> O = HBrO + H <sup>+</sup> + Br <sup>−</sup>           | 7.92                         |                         |
| Cadmium ion                     | Cd <sup>2+</sup> (aquo) hydrolysis                                                     | 9.2(1)                       |                         |
| Calcium ion                     | Ca <sup>2+</sup> (aquo) hydrolysis                                                     | 12.67(3)                     |                         |
| Californium(III) ion            | Cf <sup>3+</sup> (aquo) hydrolysis $\mu$ = 0.1                                         | 5.62                         |                         |
| Carbon dioxide                  | CO <sub>2</sub> (aquo)                                                                 | 6.352(1)                     | 10.329                  |
|                                 | CO <sub>2</sub> in D <sub>2</sub> O                                                    | 6.77                         | 10.93                   |
| Cerium(III) ion                 | Ce <sup>3+</sup> (aquo) hydrolysis                                                     | ca. 9.3                      |                         |
| Cerium(IV) ion                  | Hydrolysis to Ce(OH) <sup>3+</sup> and Ce(OH) <sub>2</sub> <sup>+</sup>                | − 1.15                       | 0.82                    |
| Chromium(III) ion               | Cr <sup>3+</sup> (aquo) hydrolysis                                                     | 3.95                         |                         |
| Cobalt(II) ion                  | Co <sup>2+</sup> (aquo) hydrolysis                                                     | 8.9                          |                         |
| Cobalt(III) ion                 | Co <sup>3+</sup> (aquo) hydrolysis $m$ = 1                                             | 1.75                         |                         |
| Copper(II) ion                  | Cu <sup>2+</sup> (aquo) hydrolysis                                                     | 7.34                         |                         |
| Curium(III) ion                 | Cm <sup>3+</sup> (aquo) hydrolysis $m$ = 0.1                                           | 6.00(5)                      |                         |
| Deuterium oxide                 | D <sub>2</sub> O (molal scale)                                                         | 14.956(1)                    |                         |
| Dysprosium(III) ion             | Dy <sup>3+</sup> (aquo) hydrolysis                                                     | 8.10                         |                         |
| Erbium(III) ion                 | Er <sup>3+</sup> (aquo) hydrolysis $\mu$ = 3                                           | 9.0                          |                         |
| Europium(III) ion               | Eu <sup>3+</sup> (aquo) hydrolysis                                                     | 8.03                         |                         |
| Fermium(III) ion                | Fm <sup>3+</sup> hydrolysis $\mu$ = 0.1                                                | 3.8                          |                         |
| Gadolinium(III) ion             | Gd <sup>3+</sup> hydrolysis                                                            | 8.27                         |                         |
| Gallium(III) ion                | Ga <sup>3+</sup> (successive values for hydrolysis)                                    | 2.92                         | 3.77                    |
|                                 |                                                                                        | p <i>K</i> <sub>3</sub> 4.75 |                         |
| Gold(III) hydroxide             | H <sub>3</sub> AuO <sub>3</sub>                                                        | < 11.7                       | 13.36                   |
| Hafnium(IV) ion                 | Hf <sup>4+</sup> hydrolysis $\mu$ = 1                                                  | − 0.12                       | 0.23                    |
| Hexaminotriphosphazene          | N <sub>3</sub> P <sub>3</sub> (NH <sub>2</sub> ) <sub>6</sub>                          | < 3.2                        | 7.68(3)                 |
| Holmium(III) ion                | Ho <sup>3+</sup> hydrolysis $\mu$ = 0.3                                                | 8.04                         |                         |

**TABLE 8.7** Proton Transfer Reactions of Inorganic Materials in Water at 25°C (*Continued*)

| Substance                                | Formula or remarks                           | pK <sub>1</sub>      | pK <sub>2</sub>      |
|------------------------------------------|----------------------------------------------|----------------------|----------------------|
| Hydrazinium(2+) ion                      | $^+H_3N-NH_3^+$                              | 0.27                 | 7.94(3)              |
| Hydrogen amidodisulfonate                | $HNSO(OH)_2$                                 | pK <sub>3</sub> 8.50 |                      |
| Hydrogen amidophosphate                  | $H_2NPO(OH)_2$ (26°C)                        | 2.739                | 8.102                |
| Hydrogen arsenate                        | $H_3AsO_4$                                   | 2.223                | 6.760                |
| Hydrogen- <i>d</i> <sub>3</sub> arsenate | $D_3AsO_4$                                   | 2.596                |                      |
| Hydrogen arsenite                        | $HAsO_2$                                     | 9.28(10)             |                      |
| Hydrogen azide                           | $HN_3$                                       | 4.62                 |                      |
| Hydrogen- <i>d</i> azide                 | $DN_3$ (in $D_2O$ )                          | 5.115                |                      |
| Hydrogen borate (3-)                     | $H_3BO_3$                                    | 9.236                |                      |
| Hydrogen bromate                         | $HBrO_3$ (in formamide)                      | 1.02                 |                      |
| Hydrogen bromide                         | $HBr$                                        | -8.72(15)            |                      |
| Hydrogen chlorate                        | $HClO_3$ (theoretical prediction)            | -2.7                 |                      |
| Hydrogen chloride                        | $HCl$                                        | -6.2(1)              |                      |
| Hydrogen- <i>d</i> chloride              | $DCl$ (in dimethylformamide)                 | 3.58                 |                      |
| Hydrogen chlorite                        | $HClO_2$                                     | 1.94                 |                      |
| Hydrogen chromate                        | $H_2CrO_4$                                   | 0.74                 | 6.488                |
| Hydrogen cyanate                         | $HOCN$                                       | 3.46                 |                      |
| Hydrogen cyanide                         | $HCN$                                        | 9.21                 |                      |
| Hydrogen- <i>d</i> cyanide               | $DCN$ (in $D_2O$ ) $\mu = 0.11$              | 8.97                 |                      |
| Hydrogen diamidophosphate                | $(NH_2)_2PO(OH)$ (30°C)                      | 1.279(+1)            | 4.889                |
| Hydrogen diamidothiophosphate            | $(NH_2)_2PO(SH)$ (20°C)                      | 2.0(+1)              | 4.3                  |
| Hydrogen diimidotriphosphate             | $(HO)_2PO(NH)PO(OH)(NH)PO(OH)_2$ $\mu = 0.1$ | $\sim 1$             | $\sim 2$             |
|                                          |                                              | pK <sub>3</sub> 3.03 | pK <sub>4</sub> 6.61 |
|                                          |                                              | pK <sub>5</sub> 9.84 |                      |
| Hydrogen diphosphate                     | $H_4P_2O_7$                                  | 0.91                 | 2.10                 |
|                                          |                                              | pK <sub>3</sub> 6.70 | pK <sub>4</sub> 9.35 |
|                                          |                                              | -12                  | -8                   |
| Hydrogen disulfate                       | $H_2S_2O_7$ (theoretical prediction)         | -3.4                 | -0.2                 |
| Hydrogen dithionate                      | $H_2S_2O_6$                                  | 0.35                 | 2.45                 |
| Hydrogen dithionite                      | $H_2S_2O_4$                                  | 3.20(4)              |                      |
| Hydrogen fluoride                        | $H_2F_2$                                     | 9.01                 | 12.30                |
| Hydrogen germanate                       | $H_2GeO_4$                                   |                      | 1.92                 |
| Hydrogen hexafluorosilicate              | $H_2SiF_6$                                   |                      | 2.50                 |
| Hydrogen hydrosulfite                    | $H_2S_2O_4$                                  | 0.35                 |                      |
| Hydrogen hypobromite                     | $HBrO$                                       | 8.55                 |                      |
| Hydrogen hypochlorite                    | $HClO$                                       | 7.537                |                      |
| Hydrogen hypoiodite                      | $HIO$                                        | 10.5(5)              |                      |
| Hydrogen hyponitrite                     | $H_2N_2O_2$                                  | 7.21                 | 11.45(10)            |
| Hydrogen iodate                          | $HIO_3$                                      | 0.804                |                      |

**Source:** J. J. Christensen, L. D. Hansen, and R. M. Izatt, *Handbook of Proton Ionization Heats and Related Thermodynamic Quantities*, Wiley-Interscience, New York, 1976; D. D. Perrin, *Ionisation Constants of Inorganic Acids and Bases in Aqueous Solution*, 2d ed., Pergamon Press, 1982.

**TABLE 8.7** Proton Transfer Reactions of Inorganic Materials in Water at 25°C (*Continued*)

| Substance                                 | Formula or remarks                                                                  | pK <sub>1</sub>          | pK <sub>2</sub>     |
|-------------------------------------------|-------------------------------------------------------------------------------------|--------------------------|---------------------|
| Hydrogen- <i>d</i> iodate                 | DIO <sub>3</sub> (in D <sub>2</sub> O)                                              | 1.15                     |                     |
| Hydrogen iodide                           | HI                                                                                  | −8.56                    |                     |
| Hydrogen manganate(VI)                    | H <sub>2</sub> MnO <sub>4</sub> (35°C) $\mu = 0.1$                                  |                          | 10.15               |
| Hydrogen nitrate                          | HNO <sub>3</sub>                                                                    | −1.37(7)                 |                     |
| Hydrogen nitrite                          | HNO <sub>2</sub>                                                                    | 3.14(1)                  |                     |
| Hydrogen perchlorate                      | HClO <sub>4</sub>                                                                   | −1.6                     |                     |
| Hydrogen periodate                        | HIO <sub>4</sub>                                                                    | 1.64                     |                     |
| Hydrogen peroxide                         | H <sub>2</sub> O <sub>2</sub>                                                       | 11.64(2)                 |                     |
| Hydrogen peroxophosphate                  | H <sub>3</sub> PO <sub>5</sub> $\mu = 0.2$                                          | 1.1                      | 5.5                 |
|                                           |                                                                                     | pK <sub>3</sub> 12.8     |                     |
| Hydrogen peroxosulfate                    | H <sub>2</sub> SO <sub>5</sub>                                                      | 1.0                      | 9.86                |
| Hydrogen perrhenate                       | HReO <sub>4</sub>                                                                   | −1.25                    |                     |
| Hydrogen pertechnetate                    | HTcO <sub>4</sub>                                                                   | 0.3                      |                     |
| Hydrogen perthiocarbonate                 | H <sub>2</sub> CS <sub>4</sub>                                                      | 3.54                     | 7.24                |
| Hydrogen perxenate                        | H <sub>4</sub> XeO <sub>6</sub>                                                     | pK <sub>3</sub> 10.5     |                     |
| Hydrogen phosphate(3−)                    | H <sub>3</sub> PO <sub>4</sub>                                                      | 2.148(20)                | 7.198(10)           |
|                                           |                                                                                     | pK <sub>3</sub> 12.32(6) |                     |
| Hydrogen- <i>d</i> <sub>2</sub> phosphate | D <sub>2</sub> PO <sub>4</sub> (in D <sub>2</sub> O)                                | 7.780                    |                     |
| Hydrogen phosphinate                      | H <sub>2</sub> PHO <sub>2</sub>                                                     | 1.23                     |                     |
| Hydrogen phosphonate                      | H <sub>2</sub> PHO <sub>3</sub>                                                     | 1.43                     | 6.68(14)            |
| Hydrogen selenate                         | H <sub>2</sub> SeO <sub>4</sub>                                                     |                          | 1.66                |
| Hydrogen selenide                         | H <sub>2</sub> Se $\mu = 0.03$                                                      | 3.89                     | 11.0                |
| Hydrogen selenite                         | H <sub>2</sub> SeO <sub>3</sub>                                                     | 2.62                     | 8.30(15)            |
| Hydrogen silicate(4−)                     | H <sub>4</sub> SiO <sub>4</sub>                                                     | 9.60(10)                 | 11.8(1)             |
| Hydrogen sulfamate                        | H <sub>2</sub> NSO <sub>3</sub> H                                                   | 0.99                     |                     |
| Hydrogen sulfate                          | H <sub>2</sub> SO <sub>4</sub>                                                      |                          | 1.99(1)             |
| Hydrogen sulfide                          | H <sub>2</sub> S                                                                    | 6.97                     | 12.90               |
| Hydrogen sulfite                          | SO <sub>2</sub> + H <sub>2</sub> O = HSO <sub>3</sub> <sup>−</sup> = H <sup>+</sup> | 1.89                     | 7.205               |
| Hydrogen tellurate                        | H <sub>6</sub> TeO <sub>6</sub>                                                     | 7.65(5)                  | 11.00(5)            |
| Hydrogen telluride                        | H <sub>2</sub> Te (18°C)                                                            | 2.64                     | 11–12               |
| Hydrogen tellurite                        | H <sub>2</sub> TeO <sub>3</sub> (20°C)                                              | 6.27                     | 8.43                |
| Hydrogen tetrafluoroborate                | BF <sub>4</sub>                                                                     | 0.5                      |                     |
| Hydrogen tetracyanonickelate              | H <sub>2</sub> Ni(CN) <sub>4</sub>                                                  | 4.69                     | 6.59                |
| Hydrogen tetraperoxochromate              | H <sub>3</sub> CrO <sub>8</sub> (30°C) $\mu = 3$                                    | 7.16                     |                     |
| Hydrogen tetrapolyphosphate               | H <sub>4</sub> P <sub>4</sub> O <sub>13</sub> $\mu = 0.034$                         | 1.99                     | 2.64                |
|                                           |                                                                                     | pK <sub>3</sub> 6.62     | pK <sub>4</sub> 8.2 |

**TABLE 8.7** Proton Transfer Reactions of Inorganic Materials in Water at 25°C (*Continued*)

| Substance                                  | Formula or remarks                                                   | pK <sub>1</sub>          | pK <sub>2</sub>      |
|--------------------------------------------|----------------------------------------------------------------------|--------------------------|----------------------|
| Hydrogen tetrathiophosphate                | H <sub>3</sub> PS <sub>4</sub>                                       | 1.5                      | 3.5                  |
| Hydrogen thiocyanate                       | HSCN $\mu = 3$                                                       | pK <sub>3</sub> 6.6      |                      |
| Hydrogen thiophosphate                     | H <sub>3</sub> PO <sub>3</sub> S                                     | −1.8                     |                      |
|                                            |                                                                      | 1.788                    | 5.427                |
| Hydrogen thiosulfate                       | H <sub>2</sub> S <sub>2</sub> O <sub>3</sub>                         | pK <sub>3</sub> 10.08    |                      |
| Hydrogen tripolyphosphate                  | H <sub>3</sub> P <sub>3</sub> O <sub>9</sub>                         | 0.6                      | 1.74                 |
|                                            |                                                                      | ~1                       | 1.7                  |
|                                            |                                                                      | pK <sub>3</sub> 2.00(10) |                      |
|                                            |                                                                      | pK <sub>4</sub> 5.83(7)  |                      |
|                                            |                                                                      | pK <sub>5</sub> 8.51(6)  |                      |
| Hydrogen triselenocarbonate                | H <sub>2</sub> CSe <sub>3</sub>                                      | 1.16                     | 7.70                 |
| Hydrogen trithiocarbonate                  | H <sub>2</sub> CS <sub>3</sub> (20°C)                                | 2.68                     | 8.18                 |
| Hydrogen tungstate                         | H <sub>2</sub> WO <sub>4</sub>                                       | 2.20                     | 3.70                 |
| Hydrogen vanadate(−1)                      | HVO <sub>3</sub>                                                     | 3.80                     |                      |
| Hydrogen vanadate(3−)                      | H <sub>3</sub> VO <sub>4</sub>                                       | 3.78                     | 7.78(4)              |
| Hydroxylamine- <i>N,N</i> -disulfonic acid | HON(SO <sub>3</sub> H) <sub>2</sub> $\mu = 1.6$                      | pK <sub>3</sub> 11.85    |                      |
| Hydroxylamine <i>O</i> -sulfonate          | <sup>+</sup> H <sub>3</sub> NOSO <sub>3</sub> <sup>−</sup> $\mu = 1$ | 1.48                     |                      |
| Imidodiphosphoric acid                     | (HO) <sub>2</sub> PO(NH)PO(OH) <sub>2</sub> $\mu = 0.2$              | ~2                       | 2.85                 |
|                                            |                                                                      | pK <sub>3</sub> 7.08     | pK <sub>4</sub> 9.72 |
| Indium(III) ion                            | In <sup>3+</sup> hydrolysis                                          | 3.54                     | 4.28                 |
| Iridium(III) ion                           | Ir <sup>3+</sup> hydrolysis $\mu = 1$                                | 4.37                     | 5.20                 |
| Iron(II) ion                               | Fe <sup>2+</sup> hydrolysis $\mu = 1$                                | 6.8                      |                      |
| Iron(III) ion                              | Fe <sup>3+</sup> hydrolysis                                          | 2.19                     |                      |
| Lanthanum(III) ion                         | La <sup>3+</sup> hydrolysis                                          | 9.06                     |                      |
| Lead(II) ion                               | Pb <sup>2+</sup> hydrolysis $\mu = 0.3$                              | 7.8                      |                      |
| Lead(IV) ion                               | Pb <sup>4+</sup> hydrolysis                                          | 1.8                      | 3.2                  |
| Lithium(I) ion                             | Li <sup>+</sup>                                                      | 13.8                     |                      |
| Lutetium(III) ion                          | Lu <sup>3+</sup> hydrolysis                                          | 7.94                     |                      |
| Magnesium(II) ion                          | Mg <sup>2+</sup> hydrolysis                                          | 11.41                    |                      |
| Manganese(II) ion                          | Mn <sup>2+</sup> hydrolysis                                          | 10.59                    |                      |
| Manganese(III) ion                         | Mn <sup>3+</sup> hydrolysis                                          | 0.4                      |                      |
| Mercury(I) ion                             | Hg <sub>2</sub> <sup>2+</sup> hydrolysis $\mu = 0.5$                 | 5.0                      |                      |
| Mercury(II) ion                            | Hg <sup>2+</sup> hydrolysis $\mu = 0.5$                              | 3.70                     | 2.65                 |
| Neodymium(III) ion                         | Nd <sup>3+</sup> hydrolysis $\mu = 3$                                | 9.0(5)                   |                      |
| Neptunium(III) ion                         | Np <sup>3+</sup> hydrolysis $\mu = 0.3$                              | 7.43                     |                      |
| Neptunium(IV) ion                          | Np <sup>4+</sup> hydrolysis $\mu = 2$                                | 2.30                     |                      |
| Neptunium(V) ion                           | NpO <sub>2</sub> <sup>+</sup> hydrolysis                             | 8.90(2)                  |                      |
| Nickel(II) ion                             | Ni <sup>2+</sup> hydrolysis                                          | 9.86                     |                      |
| Osmium tetroxide                           | OsO <sub>4</sub> hydrolysis $\mu = 1$                                | 12.1                     |                      |
| Palladium(II) ion                          | Pd <sup>2+</sup> (stepwise pK <sub>b</sub> values)                   | 13.0                     | 12.8                 |
| Pentacyanoaquoferrate(II) ion              | Fe(CN) <sub>5</sub> (H <sub>2</sub> O) <sup>3−</sup> $\mu = 0.1$     | 2.63                     |                      |

**TABLE 8.7** Proton Transfer Reactions of Inorganic Materials in Water at 25°C (*Continued*)

| Substance             | Formula or remarks                                                                    | pK <sub>1</sub>      | pK <sub>2</sub> |
|-----------------------|---------------------------------------------------------------------------------------|----------------------|-----------------|
| Plutonium(III) ion    | Pu <sup>3+</sup> hydrolysis $\mu = 0.07$                                              | 7.2(2)               |                 |
| Plutonium(IV) ion     | Pu <sup>4+</sup> hydrolysis $\mu = 2$                                                 | 1.26                 |                 |
| Plutonium(V) ion      | PuO <sub>2</sub> <sup>+</sup> hydrolysis $\mu = 0.003$                                | 9.7                  |                 |
| Plutonium(VI) ion     | PuO <sub>2</sub> <sup>2+</sup> hydrolysis                                             | 3.33                 | 4.05            |
| Polonium(IV) ion      | Po <sup>4+</sup> hydrolysis                                                           | 0.48                 | 2.74            |
|                       |                                                                                       | pK <sub>3</sub> 5.58 |                 |
| Praseodymium(III) ion | Pr <sup>3+</sup> hydrolysis $\mu = 0.3$                                               | 8.55                 |                 |
| Protoactinium(IV) ion | Pa <sup>4+</sup> hydrolysis $\mu = 3$                                                 | 0.14                 | 0.38            |
| Protoactinium(V) ion  | Pa <sup>5+</sup> hydrolysis $\mu = 3$                                                 | 1.05                 |                 |
| Scandium(III) ion     | Sc <sup>3+</sup> hydrolysis $\mu = 0.05$                                              | 4.58(3)              |                 |
| Silver(I) ion         | Ag <sup>+</sup> hydrolysis                                                            | > 11.1               |                 |
| Sodium ion            | Na <sup>+</sup> (aquo)                                                                | 14.67(10)            |                 |
| Strontium ion         | Sr <sup>2+</sup> (aquo)                                                               | 13.18                |                 |
| Terbium(III) ion      | Tb <sup>3+</sup> hydrolysis $\mu = 0.3$                                               | 8.16                 |                 |
| Thallium(I) ion       | Tl <sup>+</sup>                                                                       | 13.36(15)            |                 |
| Thallium(III) ion     | Tl <sup>3+</sup> hydrolysis $\mu = 3$                                                 | 1.14                 |                 |
| Thorium(IV) ion       | Th <sup>4+</sup> hydrolysis $\mu = 0.5$                                               | 3.89                 | 4.20            |
| Tin(II) ion           | Sn <sup>2+</sup> hydrolysis $\mu = 3$                                                 | 3.81(10)             |                 |
| Titanium(III)         | Ti <sup>3+</sup> hydrolysis $\mu = 3$                                                 | 2.55                 |                 |
| Titanium(IV)          | TiO <sub>2</sub> <sup>2+</sup> + H <sub>2</sub> O = TiO(OH) <sup>+</sup> + H          | 1.3                  |                 |
| Tritium oxide         | pK <sub>w</sub> for T <sub>2</sub> O = T <sup>+</sup> + OH <sup>-</sup>               | 15.21                |                 |
| Uranium(IV) ion       | U <sup>4+</sup> hydrolysis                                                            | 0.68                 |                 |
| Uranyl(VI) ion        | UO <sub>2</sub> <sup>2+</sup> $\mu = 0.035$                                           | 5.82                 |                 |
| Vanadium(II) ion      | V <sup>2+</sup> hydrolysis                                                            | 6.85                 |                 |
| Vanadium(III) ion     | V <sup>3+</sup> hydrolysis                                                            | 2.92                 | 3.5             |
| Vanadyl(IV) ion       | VO <sup>2+</sup> hydrolysis                                                           | 6.86(10)             |                 |
| Vanadyl(V) ion        | VO <sub>2</sub> <sup>+</sup> (20°C) $\mu = 0.1$                                       | 1.83                 |                 |
| Xenon trioxide        | XeO <sub>3</sub> + H <sub>2</sub> O = HXeO <sub>4</sub> <sup>-</sup> + H <sup>+</sup> | 10.5                 |                 |
| Ytterbium(III) ion    | Yb <sup>3+</sup> hydrolysis                                                           | 7.99(6)              |                 |
| Yttrium(III) ion      | Y <sup>3+</sup> hydrolysis $\mu = 0.3$                                                | 8.34                 |                 |
| Zinc ion              | Zn <sup>2+</sup> hydrolysis                                                           | 8.96                 |                 |
| Zirconium(IV) ion     | Zr <sup>4+</sup> hydrolysis $\mu = 1$                                                 | -0.32                | 0.06            |
|                       |                                                                                       | pK <sub>3</sub> 0.35 |                 |

If a desired organic acid is not entered in Table 8.8, a useful estimate of its  $pK_a$  value can sometimes be obtained by making a comparison with recognizably similar compounds for which  $pK_a$  values are known: (1) alkyl chains, alicyclic rings, or saturated carbocyclic rings fused to aromatic or heterocyclic rings can be replaced by methyl or ethyl groups; (2) acid-strengthening inductive and mesomeric effects of a nitro group attached to an aromatic ring are very similar to those of a nitrogen atom located at the same position in a heteroaromatic ring (e.g., 3-hydroxypyridine and 3-nitrophenol).

Hammett and Taft substituent constants and, in particular, Tables 9.1 through 9.4 may also prove useful for estimating  $pK_a$  values.

### 8.2.1.1 Calculation of the Approximate pH Value of Solutions

*Strong acid:*  $\text{pH} = -\log [\text{acid}]$

*Strong base:*  $\text{pH} = 14.00 + \log [\text{base}]$

*Weak acid:*  $\text{pH} = \frac{1}{2}pK_a - \frac{1}{2} \log [\text{acid}]$

*Weak base:*  $\text{pH} = 14.00 - \frac{1}{2}pK_b + \frac{1}{2} \log [\text{base}]$

*Salt formed by a weak acid and a strong base:*

$$\text{pH} = 7.00 + \frac{1}{2}pK_a + \frac{1}{2} \log [\text{salt}]$$

*Acid salts of a dibasic acid:*

$$\text{pH} = \frac{1}{2}pK_1 + \frac{1}{2}pK_2 - \frac{1}{2} \log [\text{salt}] + \frac{1}{2} \log (K_1 + [\text{salt}])$$

*Buffer solution consisting of a mixture of a weak acid and its salt:*

$$\text{pH} = pK_a + \log \left( \frac{[\text{salt}] + [\text{H}_3\text{O}^+] - [\text{OH}^-]}{[\text{acid}] - [\text{H}_3\text{O}^+] + [\text{OH}^-]} \right)$$

### 8.2.1.2 Calculation of Concentrations of Species Present at a Given pH

$$\begin{aligned}\alpha_0 &= \frac{[\text{H}^+]^n}{[\text{H}^+]^n + K_1[\text{H}^{+}]^{n-1} + K_1K_2[\text{H}^{+}]^{n-2} + \cdots + K_1K_2 \cdots K_n} = \frac{[\text{H}_n\text{A}]}{C_{\text{acid}}} \\ \alpha_1 &= \frac{K_1[\text{H}^+]^{n-1}}{[\text{H}^+]^n + K_1[\text{H}^{+}]^{n-1} + K_1K_2[\text{H}^{+}]^{n-2} + \cdots + K_1K_2 \cdots K_n} = \frac{[\text{H}_{n-1}\text{A}^-]}{C_{\text{acid}}} \\ \alpha_2 &= \frac{K_1K_2[\text{H}^+]^{n-2}}{[\text{H}^+]^n + K_1[\text{H}^{+}]^{n-1} + K_1K_2[\text{H}^{+}]^{n-2} + \cdots + K_1K_2 \cdots K_n} = \frac{[\text{H}_{n-2}\text{A}^{2-}]}{C_{\text{acid}}} \\ &\vdots \\ \alpha_n &= \frac{K_1K_2 \cdots K_n}{[\text{H}^+]^n + K_1[\text{H}^{+}]^{n-1} + K_1K_2[\text{H}^{+}]^{n-2} + \cdots + K_1K_2 \cdots K_n} = \frac{[\text{A}^{n-}]}{C_{\text{acid}}}\end{aligned}$$



**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C

Ionic strength  $\mu$  is zero unless otherwise indicated. Protonated cations are designated by (+1), (+ 2), etc., after the  $pK_a$  value; neutral species by (0), if not obvious; and negatively charged acids by (−1), (−2), etc.

| Substance                                                  | $pK_1$     | $pK_2$                   | $pK_3$ | $pK_4$ |
|------------------------------------------------------------|------------|--------------------------|--------|--------|
| Abietic acid                                               | 7.62       |                          |        |        |
| Acetamide                                                  | − 0.37(+1) |                          |        |        |
| Acetamidine                                                | 1.60(+1)   |                          |        |        |
| <i>N</i> -(2-Acetamido)-2-aminoethane-sulfonic acid (20°C) | 6.88       |                          |        |        |
| 2-Acetamidobenzoic acid                                    | 3.63       |                          |        |        |
| 3-Acetamidobenzoic acid                                    | 4.07       |                          |        |        |
| 4-Acetamidobenzoic acid                                    | 4.28       |                          |        |        |
| 2-(Acetamido)butanoic acid                                 | 3.716      |                          |        |        |
| <i>N</i> -(2-Acetamido)iminodiacetic acid (20°C)           | 6.62       |                          |        |        |
| 3-Acetamidopyridine                                        | 4.37(+1)   |                          |        |        |
| Acetanilide                                                | 0.4(+1)    | 13.39(0) <sup>40°C</sup> |        |        |
| Acetic acid                                                | 4.756      |                          |        |        |
| Acetic acid- <i>d</i> (in D <sub>2</sub> O)                | 5.32       |                          |        |        |
| Acetoacetic acid (18°C)                                    | 3.58       |                          |        |        |
| Acetohydrazine                                             | 3.24(+1)   |                          |        |        |
| Acetone oxime                                              | 12.2       |                          |        |        |
| 2-Acetoxybenzoic acid (acetylsalicyclic acid)              | 3.48       |                          |        |        |
| 3-Acetoxybenzoic acid                                      | 4.00       |                          |        |        |
| 4-Acetoxybenzoic acid                                      | 4.38       |                          |        |        |
| Acetylacetic acid (18°C)                                   | 3.58       |                          |        |        |
| <i>N</i> -Acetyl- $\alpha$ -alanine                        | 3.715      |                          |        |        |
| <i>N</i> -Acetyl- $\beta$ -alanine                         | 4.455      |                          |        |        |
| 2-Acetylaminobutanoic acid                                 | 3.72       |                          |        |        |
| 3-Acetylaminopropionic acid                                | 4.445      |                          |        |        |
| 2-Acetylbenzoic acid                                       | 4.13       |                          |        |        |
| 3-Acetylbenzoic acid                                       | 3.83       |                          |        |        |
| 4-Acetylbenzoic acid                                       | 3.70       |                          |        |        |
| 2-Acetylcyclohexanone                                      | 14.1       |                          |        |        |
| <i>N</i> -Acetylcysteine (30°C)                            | 9.52       |                          |        |        |
| Acetylenedicarboxylic acid                                 | 1.75       | 4.40                     |        |        |
| <i>N</i> -Acetylglycine                                    | 3.670      |                          |        |        |
| <i>N</i> -Acetylguanidine                                  | 8.23(+1)   |                          |        |        |
| <i>N</i> - $\alpha$ -Acetyl- <b>L</b> -histidine           | 7.08       |                          |        |        |
| Acetylhydroxamic acid (20°C)                               | 9.40       |                          |        |        |
| <i>N</i> -Acetyl-2-mercaptoethylamine                      | 9.92(SH)   |                          |        |        |
| 4-Acetyl- $\beta$ -mercaptoisoleucine (30°C)               | 10.30      |                          |        |        |
| 2-Acetyl-1-naphthol (30°C)                                 | 13.40      |                          |        |        |
| <i>N</i> -Acetylpenicillamine (30°C)                       | 9.90       |                          |        |        |
| 2-Acetylphenol                                             | 9.19       |                          |        |        |
| 4-Acetylphenol                                             | 8.05       |                          |        |        |
| 2-Acetylpyridine                                           | 2.643(+1)  |                          |        |        |
| 3-Acetylpyridine                                           | 3.256(+1)  |                          |        |        |
| 4-Acetylpyridine                                           | 3.505(+1)  |                          |        |        |
| Aconitine                                                  | 8.11(+1)   |                          |        |        |
| Acridine                                                   | 5.60(+1)   |                          |        |        |
| Acrylic acid                                               | 4.26       |                          |        |        |
| Adenine                                                    | 4.17(+1)   | 9.75(0)                  |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                 | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$ |
|---------------------------------------------------------------------------|-----------|-----------|-----------|--------|
| Adeninedeoxyriboside-5'-phosphoric acid                                   | —         | 4.4       | 6.4       |        |
| Adenine- <i>N</i> -oxide                                                  | 2.69(+1)  | 8.49(0)   |           |        |
| Adenosine                                                                 | 3.5(+1)   | 12.34(0)  |           |        |
| Adenosine-5'-diphosphoric acid                                            | —         | 4.2(−1)   | 7.20(−2)  |        |
| Adenosine-2'-phosphoric acid                                              | 3.81(+1)  | 6.17(0)   |           |        |
| Adenosine-3'-phosphoric acid                                              | 3.65(0)   | 5.88(−1)  |           |        |
| Adenosine-5'-phosphoric acid                                              | 3.74(0)   | 6.05(−1)  | 13.06(−2) |        |
| Adenosine-5'-triphosphoric acid                                           | —         | 4.00(−1)  | 6.48(−2)  |        |
| Adipamic acid (adipic acid monoamide)                                     | 4.629     |           |           |        |
| Adipic acid                                                               | 4.418     | 5.412     |           |        |
| $\alpha$ -Alanine                                                         | 2.34(+1)  | 9.69(0)   |           |        |
| $\beta$ -Alanine                                                          | 3.55(+1)  | 10.238(0) |           |        |
| $\alpha$ -Alanine, methyl ester ( $\mu = 0.10$ )                          | 7.743(+1) |           |           |        |
| $\beta$ -Alanine, methyl ester ( $\mu = 0.10$ )                           | 9.170(+1) |           |           |        |
| <i>N</i> - <b>D</b> -Alanyl- $\alpha$ - <b>D</b> -alanine ( $\mu = 0.1$ ) | 3.32(+1)  | 8.13(0)   |           |        |
| <i>N</i> - <b>L</b> -Alanyl- $\alpha$ - <b>L</b> -alanine ( $\mu = 0.1$ ) | 3.32(+1)  | 8.13(0)   |           |        |
| <i>N</i> - <b>L</b> -Alanyl- $\alpha$ - <b>D</b> -alanine                 | 3.12(+1)  | 8.30(0)   |           |        |
| <i>N</i> - $\alpha$ -Alanylglycine                                        | 3.11(+1)  | 8.11(0)   |           |        |
| Alanylglycylglycine                                                       | 3.190(+1) | 8.15(0)   |           |        |
| $\beta$ -Alanylhistidine                                                  | 2.64      | 6.86      | 9.40      |        |
| Albumin (bovine serum ( $\mu = 0.15$ ))                                   | 10–10.3   |           |           |        |
| 2-Aldoxime pyridine                                                       | 3.42(+1)  | 10.22(0)  |           |        |
| Alizarin Black SN                                                         | 5.79      | 12.8      |           |        |
| Alizarin-3-sulfonic acid                                                  | 5.54      | 11.01     |           |        |
| Allantoin                                                                 | 8.96      |           |           |        |
| Allothreonine                                                             | 2.108(+1) | 9.096(0)  |           |        |
| Alloxanic acid                                                            | 6.64      |           |           |        |
| Allylacetic acid                                                          | 4.68      |           |           |        |
| Allylamine                                                                | 9.69(+1)  |           |           |        |
| 5-Allylbarbituric acid                                                    | 4.78(+1)  |           |           |        |
| 5-Allyl-5-( $\alpha$ -methylbutyl)barbituric acid                         | 8.08      |           |           |        |
| 2-Allylphenol                                                             | 10.28     |           |           |        |
| 1-Allylpiperidine                                                         | 9.65(+1)  |           |           |        |
| 2-Allylpropionic acid                                                     | 4.72      |           |           |        |
| 3-Amidotetrazoline                                                        | 3.95(+1)  |           |           |        |
| 2-Aminoacetamide                                                          | 7.95(+1)  |           |           |        |
| Aminoacetonitrile                                                         | 5.34(+1)  |           |           |        |
| 9-Aminoacridine (20°C)                                                    | 9.95(+1)  |           |           |        |
| 4-Aminoantipyrene                                                         | 4.94(+1)  |           |           |        |
| 2-Aminobenzenesulfonic acid                                               | 2.459(0)  |           |           |        |
| 3-Aminobenzenesulfonic acid                                               | 3.738(0)  |           |           |        |
| 4-Aminobenzenesulfonic acid                                               | 3.227(0)  |           |           |        |
| 2-Aminobenzoic acid                                                       | 2.09(+1)  | 4.79(0)   |           |        |
| 3-Aminobenzoic acid                                                       | 3.07(+1)  | 4.79(0)   |           |        |
| 4-Aminobenzoic acid                                                       | 2.41(+1)  | 4.85(0)   |           |        |
| 2-Aminobenzoic acid, methyl ester                                         | 2.36(+1)  |           |           |        |
| 3-Aminobenzoic acid, methyl ester                                         | 3.58(+1)  |           |           |        |
| 4-Aminobenzoic acid, methyl ester                                         | 2.45(+1)  |           |           |        |
| 3-Aminobenzonitrile                                                       | 2.75(+1)  |           |           |        |
| 4-Aminobenzonitrile                                                       | 1.74(+1)  |           |           |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                             | $pK_1$    | $pK_2$    | $pK_3$   | $pK_4$ |
|-------------------------------------------------------|-----------|-----------|----------|--------|
| 4-Aminobenzophenone                                   | 2.15(+1)  |           |          |        |
| 2-Aminobenzothiazole (20°C)                           | 4.48(+1)  |           |          |        |
| 2-Aminobenzoylhydrazide                               | 1.85      | 3.47      | 12.80    |        |
| 2-Aminobiphenyl                                       | 3.78(+1)  |           |          |        |
| 3-Aminobiphenyl                                       | 4.18(+1)  |           |          |        |
| 4-Aminobiphenyl                                       | 4.27(+1)  |           |          |        |
| 4-Amino-3-bromomethylpyridine                         | 7.47(+1)  |           |          |        |
| 4-Amino-3-bromopyridine (20°C)                        | 7.04(+1)  |           |          |        |
| 2-Aminobutanoic acid                                  | 2.286(+1) | 9.830(0)  |          |        |
| 3-Aminobutanoic acid                                  | —         | 10.14(0)  |          |        |
| 4-Aminobutanoic acid                                  | 4.031(+1) | 10.556(0) |          |        |
| 2-Aminobutanoic acid, methyl ester ( $\mu = 0.1$ )    | 7.640(+1) |           |          |        |
| 4-Aminobutanoic acid, methyl ester ( $\mu = 0.1$ )    | 9.838(+1) |           |          |        |
| D-(+)-2-Amino-1-butanol                               | 9.52(+1)  |           |          |        |
| 3-Amino-N-butyl-3-methyl-2-butanone oxime             | 9.09(+1)  |           |          |        |
| 4-Aminobutylphosphonic acid                           | 2.55      | 7.55      | 10.9     |        |
| 2-Amino-N-carbamoylbutanoic acid                      | 3.886(+1) |           |          |        |
| 4-Amino-N-carbamoylbutanoic acid                      | 4.683(+1) |           |          |        |
| 2-Amino-N-carbamoyl-2-methylpropanoic acid            | 4.463     |           |          |        |
| 1-Amino-1-cycloheptanecarboxylic acid                 | 2.59(+1)  | 10.46(0)  |          |        |
| 1-Amino-1-cyclohexanecarboxylic acid                  | 2.65(+1)  | 10.03(0)  |          |        |
| 2-Amino-1-cyclohexanecarboxylic acid                  | 3.56(+1)  | 10.21(0)  |          |        |
| 1-Aminocyclopentane                                   | 10.65(+1) |           |          |        |
| 1-Aminocyclopropane                                   | 9.10(+1)  |           |          |        |
| 10-Aminodecylphosphonic acid                          | —         | 8.0       | 11.25    |        |
| 10-Aminodecylsulfonic acid                            | 2.65(+1)  |           |          |        |
| 1-Amino-2-di(aminomethyl)butane                       | 3.58(+3)  | 8.59(+2)  | 9.66(+1) |        |
| 2-Amino-N,N-dihydroxyethyl-2-hydroxyl-1,3-propanediol | 6.484(+1) |           |          |        |
| 2-Amino-N,N-dimethylbenzoic acid                      | 1.63(+1)  | 8.42(0)   |          |        |
| 4-Amino-2,5-dimethylphenol                            | 5.28(+1)  | 10.40(0)  |          |        |
| 4-Amino-3,5-dimethylpyridine (20°C)                   | 9.54(+1)  |           |          |        |
| 12-Aminododecanoic acid                               | 4.648(+1) |           |          |        |
| 2-Aminoethane-1-phosphoric acid                       | 5.838     | 10.64     |          |        |
| 1-Aminoethanesulfonic acid                            | -0.33     | 9.06      |          |        |
| 2-Aminoethanesulfonic acid                            | 1.5       | 9.061     |          |        |
| 2-Aminoethanethiol (cysteamine) ( $\mu = 0.01$ )      | 8.23(+1)  |           |          |        |
| 2-Aminoethanol (ethanolamine)                         | 9.50(+1)  |           |          |        |
| 2-[2-(2-Aminoethyl)amino-ethyl]pyridine               | 3.50      | 6.59      | 9.51     |        |
| 2-Amino-2-ethyl-1-butanol                             | 9.82(+1)  |           |          |        |
| 3-(2-Aminoethyl)indole                                | —         | 10.2      |          |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                 | $pK_1$    | $pK_2$    | $pK_3$     | $pK_4$ |
|-----------------------------------------------------------|-----------|-----------|------------|--------|
| 3-Amino- <i>N</i> -ethyl-3-methyl-2-butanone oxime        | 9.23(+1)  |           |            |        |
| <i>N</i> -(2-Aminoethyl)morpholine                        | 4.06(+2)  | 9.15(+1)  |            |        |
| <i>p</i> -(2-Aminoethyl)phenol                            | 9.3       | 10.9      |            |        |
| 2-Aminoethylphosphonic acid                               | 2.45(+1)  | 7.0(0)    | 10.8(−1)   |        |
| <i>N</i> -(2-Aminoethyl)piperidine (30°C)                 | 6.38      | 9.89      |            |        |
| 2-(2-Aminoethyl)pyridine ( $\mu = 0.5$ )                  | 4.24(+2)  | 9.78(+1)  |            |        |
| 4-Amino-3-ethylpyridine (20°C)                            | 9.51(+1)  |           |            |        |
| <i>N</i> -(2-Aminoethyl)pyrrolidine (30°C)                | 6.56(+2)  | 9.74(+1)  |            |        |
| 2-Aminofluorine                                           | 10.34(+1) |           |            |        |
| 2-Amino- <b>D</b> - $\beta$ -glucose ( $\mu = 0.05$ )     | 2.20(+1)  | 9.08(0)   |            |        |
| 2-Amino- <i>N</i> -glycylbutanoic acid                    | 3.155(+1) | 8.331(0)  |            |        |
| 7-Aminoheptanoic acid                                     | 4.502     |           |            |        |
| 2-Aminohexanoic acid                                      | 2.335(+1) | 9.834(0)  |            |        |
| 6-Aminohexanoic acid                                      | 4.373(+1) | 10.804(0) |            |        |
| <i>C</i> -Amino- <i>C</i> -hydrazinocarbonylmethane       | 2.38(+2)  | 7.69(+1)  |            |        |
| 2-Amino-3-hydroxybenzoic acid                             | 2.5(+1)   | 5.192(0)  | 10.118(OH) |        |
| <b>L</b> -2-Amino-3-hydroxybutanoic acid (threonine)      | 2.088(+1) | 9.100(0)  |            |        |
| <b>DL</b> -2-Amino-4-hydroxybutanoic acid ( $\mu = 0.1$ ) | 2.265(+1) | 9.257(0)  |            |        |
| <b>DL</b> -4-Amino-3-hydroxybutanoic acid ( $\mu = 0.1$ ) | 3.834(+1) | 9.487(0)  |            |        |
| 2-Amino-2'-hydroxydiethyl sulfide                         | 9.27(+1)  |           |            |        |
| 4-Amino-2-hydroxypyrimidine (cytosine)                    | 4.58(+1)  | 12.15(0)  |            |        |
| 3-Amino- <i>N</i> -isopropyl-3-methyl-2-butanone oxime    | 9.09(+1)  |           |            |        |
| 4-Amino-3-isopropylpyridine (20°C)                        | 9.54(+1)  |           |            |        |
| 1-Aminoisoquinoline (20°C, $\mu = 0.01$ )                 | 7.62(+1)  |           |            |        |
| 3-Aminoisoquinoline (20°C, $\mu = 0.005$ )                | 5.05(+1)  |           |            |        |
| 4-Aminoisoxazolidine-3-one                                | 7.4(+1)   |           |            |        |
| Aminomalonic acid                                         | 3.32(+1)  | 9.83(0)   |            |        |
| <b>DL</b> -2-Amino-4-mercaptoputanoic acid                | 2.22(+1)  | 8.87(0)   | 10.86(SH)  |        |
| 2-Amino-3-mercapto-3-Methylbutanoic acid                  | 1.8(+1)   | 7.9(0)    | 10.5(SH)   |        |
| 2-Amino-6-methoxybenzothiazole                            | 4.50(+1)  |           |            |        |
| 3-Amino-4-methylbenzenesulfonic acid                      | 3.633     |           |            |        |
| 4-Amino-3-methylbenzenesulfonic acid                      | 3.125     |           |            |        |
| 2-Amino-4-methylbenzothiazole                             | 4.7(+1)   |           |            |        |
| 1-Amino-3-methylbutane                                    | 10.64(+1) |           |            |        |
| 3-Amino-3-methyl-2-butanone oxime                         | 9.09(+1)  |           |            |        |
| 3-Amino- <i>N</i> -methyl-3-methyl-2-butanone oxime       | 9.23(+1)  |           |            |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                | $pK_1$    | $pK_2$    | $pK_3$ | $pK_4$ |
|------------------------------------------|-----------|-----------|--------|--------|
| 2-Amino-3-methylpentanoic acid           | 2.320(+1) | 9.758(0)  | 10.8   |        |
| 3-Aminomethyl-6-methylpyridine (30°C)    | 8.70(+1)  |           |        |        |
| Aminomethylphosphonic acid               | 2.35      | 5.9       |        |        |
| 2-Amino-2-methyl-1,3-propanediol         | 8.801     |           |        |        |
| 2-Amino-2-methyl-1-propanol              | 9.694(+1) |           |        |        |
| 2-Amino-2-methylpropanoic acid           | 2.357(+1) | 10.205(0) |        |        |
| (2-Aminomethyl(pyridine ( $\mu = 0.5$ )) | 2.31(+2)  | 8.79(+1)  |        |        |
| 2-Amino-3-methylpyridine                 | 7.24(+1)  |           |        |        |
| 4-Amino-3-methylpyridine                 | 9.43(+1)  |           |        |        |
| 2-Amino-4-methylpyridine                 | 7.48(+1)  |           |        |        |
| 2-Amino-5-methylpyridine                 | 7.22(+1)  |           |        |        |
| 2-Amino-6-methylpyridine                 | 7.41(+1)  |           |        |        |
| 2-Amino-4-methylpyrimidine (20°C)        | 4.11(+1)  |           |        |        |
| Aminomethylsulfonic acid                 | 5.57(+1)  |           |        |        |
| N-Aminomorpholine                        | 4.19(+1)  |           |        |        |
| 4-Amino-1-naphthalenesulfonic acid       | 2.81      |           |        |        |
| 1-Amino-2-naphthalenesulfonic acid       | 1.71      |           |        |        |
| 1-Amino-3-naphthalenesulfonic acid       | 3.20      |           |        |        |
| 1-Amino-5-naphthalenesulfonic acid       | 3.69      |           |        |        |
| 1-Amino-6-naphthalenesulfonic acid       | 3.80      |           |        |        |
| 1-Amino-7-naphthalenesulfonic acid       | 3.66      |           |        |        |
| 1-Amino-8-naphthalenesulfonic acid       | 5.03      |           |        |        |
| 2-Amino-1-naphthalenesulfonic acid       | 2.35      |           |        |        |
| 2-Amino-4-naphthalenesulfonic acid       | 3.79      |           |        |        |
| 2-Amino-6-naphthalenesulfonic acid       | 3.79      | 8.94      |        |        |
| 2-Amino-8-naphthalenesulfonic acid       | 3.89      |           |        |        |
| 3-Amino-1-naphthoic acid                 | 2.61      | 4.39      |        |        |
| 4-Amino-2-naphthoic acid                 | 2.89      | 4.46      |        |        |
| 8-Amino-2-naphthol                       | 4.20(+1)  |           |        |        |
| DL-2-Aminopentanoic acid (DL-norvaline)  | 2.318(+1) | 9.808     |        |        |
| 3-Aminopentanoic acid                    | 4.02(+1)  | 10.399(0) |        |        |
| 4-Aminopentanoic acid                    | 3.97(+1)  | 10.46(0)  |        |        |
| 5-Aminopentanoic acid                    | 4.20(+1)  | 9.758(0)  |        |        |
| 5-Aminopentanoic acid, ethyl ester       | 10.151    |           |        |        |
| 2-Aminophenol                            | 9.28      | 9.72      |        |        |
| 3-Aminophenol                            | 9.83      | 9.87      |        |        |
| 4-Aminophenol                            | 8.50      | 10.30     |        |        |
| 4-Aminophenylacetic acid (20°C)          | 3.60      | 5.26      |        |        |
| 2-Aminophenylarsonic acid                | ca 2      | 3.77      | 8.66   |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                               | $pK_1$    | $pK_2$    | $pK_3$   | $pK_4$   |
|---------------------------------------------------------|-----------|-----------|----------|----------|
| 3-Aminophenylarsonic acid                               | ca 2      | 4.02      | 8.92     | 9.82(−2) |
| 4-Aminophenylarsonic acid                               | ca 2      | 4.02      | 8.62     |          |
| 3-Aminophenylboric acid                                 | 4.46      | 8.81      |          |          |
| 4-Aminophenylboric acid                                 | 3.71      | 9.17      |          |          |
| 4-Aminophenyl (4-chlorophenyl) sulfone                  | 1.38      |           |          |          |
| 2-Aminophenylphosphonic acid                            | —         | 4.10      | 7.29     |          |
| 3-Aminophenylphosphonic acid                            | —         | —         | 7.16     |          |
| 4-Aminophenylphosphonic acid                            | —         | —         | 7.53     |          |
| 1-Amino-1,2,3-propanetricarboxylic acid ( $\mu = 2.2$ ) | 2.10(+1)  | 3.60(0)   | 4.60(−1) |          |
| 3-Aminopropanoic acid                                   | 3.551(+1) | 10.235(0) |          |          |
| 1-Amino-1-propanol                                      | 9.96(+1)  |           |          |          |
| DL-2-Amino-1-propanol                                   | 9.469(+1) |           |          |          |
| 3-Amino-1-propanol                                      | 9.96(+1)  |           |          |          |
| 3-Aminopropene                                          | 9.691(+1) |           |          |          |
| 3-Amino- <i>N</i> -propyl-3-methyl-2-butanone oxime     | 9.09(+1)  |           |          |          |
| 2-Aminopropylsulfonic acid                              | —         | 9.15      |          |          |
| 2-Aminopyridine                                         | 6.71(+1)  |           |          |          |
| 3-Aminopyridine                                         | 6.03(+1)  |           |          |          |
| 4-Aminopyridine                                         | 9.114(+1) |           |          |          |
| 2-Aminopyridine-1-oxide                                 | 2.58(+1)  |           |          |          |
| 3-Aminopyridine-1-oxide                                 | 1.47(+1)  |           |          |          |
| 4-Aminopyridine-1-oxide                                 | 3.54(+1)  |           |          |          |
| 8-Aminoquinaldine                                       | 4.86(+1)  |           |          |          |
| 2-Aminoquinoline (20°C, $\mu = 0.01$ )                  | 7.34(+1)  |           |          |          |
| 3-Aminoquinoline (20°C, $\mu = 0.01$ )                  | 4.95(+1)  |           |          |          |
| 4-Aminoquinoline (20°C, $\mu = 0.01$ )                  | 9.17(+1)  |           |          |          |
| 5-Aminoquinoline (20°C, $\mu = 0.01$ )                  | 5.46(+1)  |           |          |          |
| 6-Aminoquinoline (20°C, $\mu = 0.01$ )                  | 5.63(+1)  |           |          |          |
| 8-Aminoquinoline (20°C, $\mu = 0.01$ )                  | 3.99(+1)  |           |          |          |
| 4-Aminosalicyclic acid                                  | 1.991(+1) | 3.917(0)  | 13.74    |          |
| 5-Aminosalicyclic acid                                  | 2.74(+1)  | 5.84(0)   |          |          |
| 2-Amino-3-sulfopropanoic acid                           | 1.89(+1)  | 8.70(0)   |          |          |
| 4-Amino-2,3,5,6-tetramethylpyridine (20°C)              | 10.58(+1) |           |          |          |
| 5-Amino-1,2,3,4-tetrazole (20°C)                        | 1.76      | 6.07      |          |          |
| 2-Aminothiazole (20°C)                                  | 5.36(+1)  |           |          |          |
| 1-Amino-3-thiobutane (30°C)                             | 9.18(+1)  |           |          |          |
| 5-Amino-3-thio-1-pentanol (30°C)                        | 9.12(+1)  |           |          |          |
| 2-Aminothiophenol                                       | <2(+1)    | 7.90(0)   |          |          |
| 2-Amino-4,4,4-trifluorobutanoic acid                    |           | 8.171(0)  |          |          |
| 3-Amino-4,4,4-trifluorobutanoic acid                    |           | 5.831(0)  |          |          |
| 3-Amino-2,4,6-trinitrobenzene                           |           | 9.5(+1)   |          |          |
| Angiotensin II                                          | 10.37     |           |          |          |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                        | $pK_1$    | $pK_2$      | $pK_3$    | $pK_4$    |
|--------------------------------------------------|-----------|-------------|-----------|-----------|
| Anhydroplatynecine                               | 9.40      |             |           |           |
| Aniline                                          | 4.60(+1)  |             |           |           |
| 2-Anilinoethylsulfonic acid                      | 3.80(+1)  |             |           |           |
| 3-Anilinoethylsulfonic acid                      | 4.85(+1)  |             |           |           |
| Anthracene-1-carboxylic acid                     | 3.68      |             |           |           |
| Anthracene-2-carboxylic acid                     | 4.18      |             |           |           |
| Anthracene-9-carboxylic acid                     | 3.65      |             |           |           |
| Anthraquinone-1-carboxylic acid (20°C)           | 3.37      |             |           |           |
| Anthraquinone-2-carboxylic acid (20°C)           | 3.42      |             |           |           |
| 9,10-Anthraquinone monoxime                      | 9.78      |             |           |           |
| 9,10-Anthraquinone-1-sulfonic acid               | 0.27      |             |           |           |
| 9,10-Anthraquinone-2-sulfonic acid               | 0.38      |             |           |           |
| Antipyrine                                       | 1.45(+1)  |             |           |           |
| Apomorphine (15°C)                               |           | 8.92        |           |           |
| D-(−)-Arabinose                                  | 12.34     |             |           |           |
| L-(+)-Arginine                                   | 2.17      | 9.04(+1)    | 12.47(−1) |           |
| Arsenazo III [ $pK_5$ 10.5(−4); $pK_6$ 12.0(−5)] |           | 1.2         | 2.7       | 7.9(−3)   |
| Arsenoacetic acid                                |           | 4.67        | 7.68      |           |
| Arsenoacrylic acid                               |           | 4.23        | 8.60      |           |
| Arsenobutanoic acid                              |           | 4.92        | 7.64      |           |
| 2-Arsenocrotonic acid                            |           | 4.61        | 8.75      |           |
| 3-Arsenocrotonic acid                            |           | 4.03        | 8.81      |           |
| Arsenopentanoic acid                             |           | 4.89        | 7.75      |           |
| L-(+)-Ascorbic acid (vitamin C)                  | 4.17      | 11.57       |           |           |
| L-(+)-Asparagine                                 | 2.01(0)   | 8.80(+1)    |           |           |
| L-Asparaginyglycine                              |           | 4.53        | 9.07      |           |
| D-Aspartic acid                                  | 1.89(0)   | 3.65        | 9.60      |           |
| Aspartic diamide ( $\mu = 0.2$ )                 | 7.00      |             |           |           |
| Aspartylaspartic acid                            |           | 3.40        | 4.70      | 8.26      |
| $\alpha$ -Aspartylhistidine (38°C, $\mu = 0.1$ ) |           | 3.02        | 6.82      | 7.98      |
| $\beta$ -Aspartylhistidine (38°C, $\mu = 0.1$ )  |           | 2.95        | 6.93      | 8.72      |
| N-Aspartyl-p-tyrosine ( $\mu = 0.01$ )           |           | 3.57        | 8.92      | 10.23(OH) |
| Aspidospermine                                   | 7.65      |             |           |           |
| Atropine (17°C)                                  | 4.35(+1)  |             |           |           |
| 1-Azacycloheptane                                | 11.11(+1) |             |           |           |
| 1-Azacyclooctane                                 | 11.1(+1)  |             |           |           |
| Azetidine                                        | 11.29(+1) |             |           |           |
| Aziridine                                        | 8.04(+1)  |             |           |           |
| Barbituric acid                                  |           | 8.372(0)    |           |           |
| m-Benzetaine                                     | 3.217(+1) |             |           |           |
| p-Benzetaine                                     | 3.245(+1) |             |           |           |
| Benzenearsonic acid (22°C)                       |           | 8.48(−1)    |           |           |
| Benzene-1-arsonic acid-4-carboxylic acid         |           | 4.22 (COOH) | 5.59      |           |
| Benzeneboronic acid                              | 13.7      |             |           |           |
| Benzene-1-carboxylic acid-2-phosphoric acid      |           | 3.78        | 9.17      |           |
| Benzene-1-carboxylic acid-3-phosphoric acid      |           | 4.03        | 7.03      |           |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                             | $pK_1$     | $pK_2$    | $pK_3$ | $pK_4$ |
|-------------------------------------------------------|------------|-----------|--------|--------|
| Benzene-1-carboxylic acid-4-phosphoric acid           | 1.50       | 3.95      | 6.89   |        |
| Benzenediazine                                        | 11.08(+1)  |           |        |        |
| 1,3-Benzenedicarboxylic acid (isophthalic acid)       | 3.62(0)    | 4.60(−1)  |        |        |
| 1,4-Benzenedicarboxylic acid (terephthalic acid)      | 3.54(0)    | 4.46(−1)  |        |        |
| 1,3-Benzenedicarboxylic acid mononitrile              | 3.60(0)    |           |        |        |
| 1,4-Benzenedicarboxylic acid mononitrile              | 3.55(0)    |           |        |        |
| Benzenhexacarboxylic acid ( $pK_5$ 6.32; $pK_6$ 7.49) | 0.68       | 2.21      | 3.52   | 5.09   |
| Benzenepentacarboxylic acid ( $pK_5$ 6.46)            | 1.80       | 2.73      | 3.96   | 5.25   |
| Benzenesulfinic acid                                  | 1.50       |           |        |        |
| Benzenesulfonic acid                                  | 2.554      |           |        |        |
| 1,2,3,4-Benzenetetracarboxylic acid                   | 2.05       | 3.25      | 4.73   | 6.21   |
| 1,2,3,5-Benzenetetracarboxylic acid                   | 2.38       | 3.51      | 4.44   | 5.81   |
| 1,2,4,5-Benzenetetracarboxylic acid                   | 1.92       | 2.87      | 4.49   | 5.63   |
| 1,2,3-Benzenetricarboxylic acid                       | 2.88       | 4.75      | 7.13   |        |
| 1,2,4-Benzenetricarboxylic acid                       | 2.52       | 3.84      | 5.20   |        |
| 1,3,5-Benzenetricarboxylic acid                       | 2.12       | 4.10      | 5.18   |        |
| Benzil- $\alpha$ -dioxime                             | 12.0       |           |        |        |
| Benzilic acid                                         | 3.09       |           |        |        |
| Benzimidazole                                         | 5.53(+1)   | 12.3(0)   |        |        |
| Benzohydroxamic acid (20°C)                           | 8.89(0)    |           |        |        |
| Benzoic acid                                          | 4.204      |           |        |        |
| 5,6-Benzoquinoline (20°C)                             | 5.00(+1)   |           |        |        |
| 7,8-Benzoquinoline (20°C)                             | 4.15(+1)   |           |        |        |
| 1,4-Benzoquinone monoxime                             | 6.20       |           |        |        |
| Benzosulfonic acid                                    | 0.70       |           |        |        |
| 1,2,3-Benzotriazole                                   | 8.38(+1)   |           |        |        |
| 1-Benzoylacetone                                      | 8.23       |           |        |        |
| Benzoylamine                                          | 9.34(+1)   |           |        |        |
| 2-Benzoylbenzoic acid                                 | 3.54       |           |        |        |
| Benzoylglutamic acid                                  | 3.49       | 4.99      |        |        |
| N-Benzoyglycine (hippuric acid)                       | 3.65       |           |        |        |
| Benzoylhydrazine                                      | 3.03(+2)   | 12.45(+1) |        |        |
| Benzoylpyruvic acid                                   | 6.40       | 12.10     |        |        |
| 3-Benzoyl-1,1,1-trifluoroacetone                      | 6.35       |           |        |        |
| Benzylamine                                           | 9.35(+1)   |           |        |        |
| Benzylamine-4-carboxylic acid                         | 3.59       | 9.64      |        |        |
| 2-Benzyl-2-phenylsuccinic acid (20°C)                 | 3.69       | 6.47      |        |        |
| 2-Benzylpyridine                                      | 5.13(+1)   |           |        |        |
| 4-Benzylpyridine-1-oxide                              | −1.018(+1) |           |        |        |
| 1-Benzylpyrrolidine                                   | 9.51(+1)   |           |        |        |
| 2-Benzylpyrrolidine                                   | 10.31(+1)  |           |        |        |
| Benzylsuccinic acid (20°C)                            | 4.11       | 5.65      |        |        |
| 3-(Benzylthio)propanoic acid                          | 4.463      |           |        |        |
| Berberine (18°C)                                      | 11.73(+1)  |           |        |        |
| Betaine                                               | 1.832(+1)  |           |        |        |



TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                                                        | $pK_1$    | $pK_2$    | $pK_3$   | $pK_4$   |
|----------------------------------------------------------------------------------|-----------|-----------|----------|----------|
| Biguanide                                                                        | 2.96(+2)  | 11.51(+1) |          |          |
| 2,2'-Biimidazolyl ( $\mu = 0.3$ )                                                | 5.01(+1)  |           |          |          |
| 2-Biphenylcarboxylic acid                                                        | 3.46      |           |          |          |
| (1,1'-Biphenyl)-4,4'-diamine                                                     | 3.63(+2)  | 4.70(+1)  |          |          |
| Bis(2-aminoethyl) ether (30°C)                                                   | 8.62(+2)  | 9.59(+1)  |          |          |
| <i>N,N'</i> -Bis(2-aminoethyl)-ethylenedi-<br>amine (20°C)                       | 3.32(+4)  | 6.67(+3)  | 9.20(+2) | 9.92(+1) |
| <i>N,N</i> -Bis(2-hydroxyethyl)-2-ami-<br>noethane sulfonic acid (BES)<br>(20°C) | 7.15      |           |          |          |
| <i>N,N</i> -Bis(2-hydroxyethyl)glycine<br>(bicine) (20°C)                        | 8.35      |           |          |          |
| Bis(2-hydroxyethyl)iminotris (hy-<br>droxymethyl)methane (bis-tris)              | 6.46(+1)  |           |          |          |
| 1,3-Bis[tris(hydroxymethyl)methyl-<br>lamino]propane (20°C)                      | 6.80(+1)  |           |          |          |
| Bromoacetic acid                                                                 | 2.902     |           |          |          |
| 2-Bromoaniline                                                                   | 2.53(+1)  |           |          |          |
| 3-Bromoaniline                                                                   | 3.53(+1)  |           |          |          |
| 4-Bromoaniline                                                                   | 3.88(+1)  |           |          |          |
| 2-Bromobenzoic acid                                                              | 2.85      |           |          |          |
| 3-Bromobenzoic acid                                                              | 3.810     |           |          |          |
| 4-Bromobenzoic acid                                                              | 3.99      |           |          |          |
| 2-Bromobutanoic acid (35°C)                                                      | 2.939     |           |          |          |
| <i>erythro</i> -2-Bromo-3-chlorosuccinic<br>acid (19°C, $\mu = 0.1$ )            | 1.4       | 2.6       |          |          |
| <i>threo</i> -2-Bromo-chlorosuccinic acid<br>(19°C, $\mu = 0.1$ )                | 1.5       | 2.8       |          |          |
| <i>trans</i> -2-Bromocinnamic acid                                               | 4.41      |           |          |          |
| 3-Bromo-4-(dimethylam-<br>ino)pyridine (20°C)                                    | 6.52(+1)  |           |          |          |
| 2-Bromo-4,6-dinitroaniline                                                       | -6.94(+1) |           |          |          |
| 3-Bromo-2-hydroxymethylbenzoic<br>acid (20°C)                                    | 3.28      |           |          |          |
| 6-Bromo-2-hydroxymethylbenzoic<br>acid (20°C)                                    | 2.25      |           |          |          |
| 7-Bromo-8-hydroxyquinoline-5-<br>sulfonic acid                                   | 2.51      | 6.70      |          |          |
| 3-Bromomandelic acid                                                             | 3.13      |           |          |          |
| 3-Bromo-4-methylaminopyridine<br>(20°C)                                          | 7.49(+1)  |           |          |          |
| (2-Bromomethyl)butanoic acid                                                     | 3.92      |           |          |          |
| Bromomethylphosphonic acid                                                       | 1.14      | 6.52      |          |          |
| 2-Bromo-6-nitrobenzoic acid                                                      | 1.37      |           |          |          |
| 2-Bromophenol                                                                    | 8.452     |           |          |          |
| 3-Bromophenol                                                                    | 9.031     |           |          |          |
| 4-Bromophenol                                                                    | 9.34      |           |          |          |
| 2-(2'-Bromophenoxy)acetic acid                                                   | 3.12      |           |          |          |
| 2-(3'-Bromophenoxy)acetic acid                                                   | 3.09      |           |          |          |
| 2-(4'-Bromophenoxy)acetic acid                                                   | 3.13      |           |          |          |
| 2-Bromo-2-phenylacetic acid                                                      | 2.21      |           |          |          |
| 2-(Bromophenyl) acetic acid                                                      | 4.054     |           |          |          |
| 4-(Bromophenyl)acetic acid                                                       | 4.188     |           |          |          |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                      | $pK_1$     | $pK_2$    | $pK_3$ | $pK_4$ |
|--------------------------------------------------------------------------------|------------|-----------|--------|--------|
| 4-Bromophenylarsonic acid                                                      | 3.25       | 8.19      |        |        |
| 4-Bromophenylphosphinic acid<br>(17°C)                                         | 2.1        |           |        |        |
| 2-Bromophenylphosphonic acid                                                   | 1.64       | 7.00      |        |        |
| 3-Bromophenylphosphonic acid                                                   | 1.45       | 6.69      |        |        |
| 4-Bromophenylphosphonic acid                                                   | 1.60       | 6.83      |        |        |
| 3-Bromophenylselenic acid                                                      | 4.43       |           |        |        |
| 4-Bromophenylselenic acid                                                      | 4.50       |           |        |        |
| 2-Bromopropanoic acid                                                          | 2.971      |           |        |        |
| 3-Bromopropanoic acid                                                          | 3.992      |           |        |        |
| Bromopropynoic acid                                                            | 1.855      |           |        |        |
| 2-Bromopyridine                                                                | 0.71(+1)   |           |        |        |
| 3-Bromopyridine                                                                | 2.85(+1)   |           |        |        |
| 4-Bromopyridine                                                                | 3.71(+1)   |           |        |        |
| 3-Bromoquinoline                                                               | 2.69(+1)   |           |        |        |
| Bromosuccinic acid                                                             | 2.55       | 4.41      |        |        |
| 2-Bromo- <i>p</i> -tolylphosphonic acid                                        | 1.81       | 7.15      |        |        |
| Brucine (15°C)                                                                 | 2.50(+2)   | 8.16(+1)  |        |        |
| 2-Butanamine ( <i>sec</i> -butylamine)                                         | 10.56(+1)  |           |        |        |
| 1,2-Butanediamine                                                              | 6.399(+2)  | 9.388(+1) |        |        |
| 1,4-Butanediamine                                                              | 9.35(+2)   | 10.82(+1) |        |        |
| 2,3-Butanediamine                                                              | 6.91(+2)   | 10.00(+1) |        |        |
| 1,2,3,4-Butanetetra-carboxylic acid                                            | 3.43       | 4.58      | 5.85   | 7.16   |
| <i>cis</i> -2-Butenoic acid ( <i>isocrotonic</i><br>acid)                      | 4.44       |           |        |        |
| <i>trans</i> -2-Butenoic acid ( <i>trans-cro-</i><br><i>tonic</i> acid) (35°C) | 4.676      |           |        |        |
| 3-Butenoic acid (vinylacetic acid)                                             | 4.68       |           |        |        |
| 3-Butoxybenzoic acid (20°C)                                                    | 4.25       |           |        |        |
| Butylamine                                                                     | 10.64(+1)  |           |        |        |
| <i>tert</i> -Butylamine                                                        | 10.685(+1) |           |        |        |
| 4- <i>tert</i> -Butylaniline                                                   | 3.78(+1)   |           |        |        |
| <i>N-tert</i> -Butylaniline                                                    | 7.10(+1)   |           |        |        |
| Butylarsonic acid (18°C)                                                       | 4.23       | 8.91      |        |        |
| 2- <i>tert</i> -Butylbenzoic acid                                              | 3.57       |           |        |        |
| 3- <i>tert</i> -Butylbenzoic acid                                              | 4.199      |           |        |        |
| 4- <i>tert</i> -Butylbenzoic acid                                              | 4.389      |           |        |        |
| <i>N</i> -Butylethylenediamine                                                 | 7.53(+2)   | 10.30(+1) |        |        |
| <i>N</i> -Butylglycine                                                         | 2.35(+1)   | 10.25(0)  |        |        |
| <i>tert</i> -Butylhydroperoxide                                                | 12.80      |           |        |        |
| 1-( <i>tert</i> -Butyl)-2-hydroxybenzene                                       | 10.62      |           |        |        |
| 1-( <i>tert</i> -Butyl)-3-hydroxybenzene                                       | 10.119     |           |        |        |
| 1-( <i>tert</i> -Butyl)-4-hydroxybenzene                                       | 10.23      |           |        |        |
| Butylmethylamine                                                               | 10.90(+1)  |           |        |        |
| 2-Butyl-1-methyl-2-pyrroline                                                   | 11.84(+1)  |           |        |        |
| 4- <i>tert</i> -Butylphenylactic acid                                          | 4.417      |           |        |        |
| Butylphosphinic acid                                                           | 3.41       |           |        |        |
| <i>tert</i> -Butylphosphinic acid                                              | 4.24       |           |        |        |
| <i>tert</i> -Butylphosphonic acid                                              | 2.79       | 8.88      |        |        |
| 1-Butylpiperidine ( $\mu = 0.02$ )                                             | 10.43(+1)  |           |        |        |
| 2- <i>tert</i> -Butylpyridine                                                  | 5.76(+1)   |           |        |        |
| 3- <i>tert</i> -Butylpyridine                                                  | 5.82(+1)   |           |        |        |
| 4- <i>tert</i> -Butylpyridine                                                  | 5.99(+1)   |           |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                       | $pK_1$    | $pK_2$   | $pK_3$  | $pK_4$ |
|-------------------------------------------------|-----------|----------|---------|--------|
| 2- <i>tert</i> -Butylthiazole ( $\mu = 0.1$ )   | 3.00(+1)  |          |         |        |
| 4- <i>tert</i> -Butylthiazole ( $\mu = 0.1$ )   | 3.04(+1)  |          |         |        |
| 2-Butyn-1,4-dioic acid                          | 1.75      | 4.40     |         |        |
| 2-Butynoic acid (tetrolic acid)                 | 2.620     |          |         |        |
| Butyric acid                                    | 4.817     |          |         |        |
| 4-Butyrobetaine (20°C)                          | 3.94(+1)  |          |         |        |
| Caffeine (40°C)                                 | 10.4      |          |         |        |
| Calcein ( $pK_5 > 12$ )                         | <4        |          | 9.0     | 10.5   |
| Calmagite                                       | 8.14      | 12.35    |         |        |
| D-Camphoric acid                                | 4.57      | 5.10     |         |        |
| Canaline                                        | 2.40      | 3.70     | 9.20    |        |
| Canavanine                                      | 2.50(+2)  | 6.60(+1) | 9.25(0) |        |
| N-Carbamoylacetic acid                          | 3.64      |          |         |        |
| N-Carbamoyl- $\alpha$ -D-alanine                | 3.89(+1)  |          |         |        |
| N-Carbamoyl- $\beta$ -alanine                   | 4.99(+1)  |          |         |        |
| DL-N-Carbamoylalanine                           | 3.892(+1) |          |         |        |
| N-Carbamoylglycine                              | 3.876     |          |         |        |
| 2-Carbamoylpyridine (20°C)                      | 2.10(+1)  |          |         |        |
| 3-Carbamoylpyridine                             | 3.328(+1) |          |         |        |
| 4-Carbamoylpyridine (20°C)                      | 3.61(+1)  |          |         |        |
| $\beta$ -Carboxymethylaminopropanoic acid       | 3.61(+1)  | 9.46(0)  |         |        |
| Chloroacetic acid                               | 2.867     |          |         |        |
| N-(2'-Chloroacetyl)glycine                      | 3.38(0)   |          |         |        |
| cis-3-Chloroacrylic acid (18°C, $\mu = 0.1$ )   | 3.32      |          |         |        |
| trans-3-chloroacrylic acid (18°C, $\mu = 0.1$ ) | 3.65      |          |         |        |
| 2-Chloroaniline                                 | 2.64(+1)  |          |         |        |
| 3-Chloroaniline                                 | 3.52(+1)  |          |         |        |
| 4-Chloroaniline                                 | 3.99(+1)  |          |         |        |
| 2-Chlorobenzoic acid                            | 2.877     |          |         |        |
| 3-Chlorobenzoic acid                            | 3.83      |          |         |        |
| 4-Chlorobenzoic acid                            | 3.986     |          |         |        |
| 2-Chlorobutanoic acid                           | 2.86      |          |         |        |
| 3-Chlorobutanoic acid                           | 4.05      |          |         |        |
| 4-Chlorobutanoic acid                           | 4.50      |          |         |        |
| 2-Chloro-3-butenic acid                         | 2.54      |          |         |        |
| 3-Chlorobutylarsonic acid (18°C)                | 3.95      | 8.85     |         |        |
| trans-2'-Chlorocinnamic acid                    | 4.234     |          |         |        |
| trans-3'-Chlorocinnamic acid                    | 4.294     |          |         |        |
| trans-4'-Chlorocinnamic acid                    | 4.413     |          |         |        |
| 2-Chlorocrotonic acid                           | 3.14      |          |         |        |
| 3-Chlorocrotonic acid                           | 3.84      |          |         |        |
| Chlorodifluoroacetic acid                       | 0.46      |          |         |        |
| 1-Chloro-1,2-dihydroxybenzene                   | 8.522     |          |         |        |
| 1-Chloro-2,6-dimethyl-4-hydroxybenzene          | 9.549     |          |         |        |
| 4-Chloro-2,6-dinitrophenol                      | 2.97      |          |         |        |
| 2-Chloroethylarsonic acid                       | 3.68      | 8.37     |         |        |
| 3-Chlorohexyl-1-arsonic acid (18°C)             | 3.51      | 8.31     |         |        |
| 2-Chloro-3-hydroxybutanoic acid                 | 2.59      |          |         |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                      | $pK_1$    | $pK_2$  | $pK_3$ | $pK_4$ |
|------------------------------------------------|-----------|---------|--------|--------|
| 3-Chloro-2-(hydroxy-methyl)benzoic acid (20°C) | 3.27      |         |        |        |
| 6-Chloro-2-(hydroxy-methyl)benzoic acid (20°C) | 2.26      |         |        |        |
| 7-Chloro-8-hydroxyquinoline-5-sulfonic acid    | 2.92      | 6.80    |        |        |
| 2-Chloroisocrotonic acid                       | 2.80      |         |        |        |
| 3-Chloroisocrotonic acid                       | 4.02      |         |        |        |
| 3-Chlorolactic acid                            | 3.12      |         |        |        |
| 3-Chloromandelic acid                          | 3.237     |         |        |        |
| 3-Chloro-4-methoxyphenyl-phosphonic acid       | 2.25      | 6.7     |        |        |
| 3-Chloro-4-methylaniline                       | 4.05(+1)  |         |        |        |
| 4-Chloro- <i>N</i> -methylaniline              | 3.9(+1)   |         |        |        |
| 4-Chloro-3-methylphenol                        | 9.549     |         |        |        |
| Chloromethylphosphonic acid                    | 1.40      | 6.30    |        |        |
| 2-Chloro-2-methylpropanoic acid                | 2.975     |         |        |        |
| 2-Chloro-6-nitroaniline                        | -2.41(+1) |         |        |        |
| 4-Chloro-2-nitroaniline                        | -1.10(+1) |         |        |        |
| 2-Chloro-3-nitrobenzoic acid                   | 2.02      |         |        |        |
| 2-Chloro-4-nitrobenzoic acid                   | 1.96      |         |        |        |
| 2-Chloro-5-nitrobenzoic acid                   | 2.17      |         |        |        |
| 2-Chloro-6-nitrobenzoic acid                   | 1.342     |         |        |        |
| 4-Chloro-2-nitrophenol                         | 6.48      |         |        |        |
| 2-Chlorophenol                                 | 8.55      |         |        |        |
| 3-Chlorophenol                                 | 9.10      |         |        |        |
| 4-Chlorophenol                                 | 9.43      |         |        |        |
| (4-Chloro-3-nitrophenoxy)acetic acid           | 2.959     |         |        |        |
| 2-Chloro-4-nitrophenylphosphonic acid          | 1.12      | 6.14    |        |        |
| 3-Chloropentyl-1-arsonic acid (18°C)           | 3.71      | 8.77    |        |        |
| 2-Chlorophenoxyacetic acid                     | 3.05      |         |        |        |
| 3-Chlorophenoxyacetic acid                     | 3.07      |         |        |        |
| 4-Chlorophenoxyacetic acid                     | 3.10      |         |        |        |
| 4-Chlorophenoxy-2-methylacetic acid            | 3.26      |         |        |        |
| 2-Chlorophenylacetic acid                      | 4.066     |         |        |        |
| 3-Chlorophenylacetic acid                      | 4.140     |         |        |        |
| 4-Chlorophenylacetic acid                      | 4.190     |         |        |        |
| 2-Chlorophenylalanine                          | 2.23(+1)  | 8.94(0) |        |        |
| 3-Chlorophenylalanine                          | 2.17(+1)  | 8.91(0) |        |        |
| <b>DL</b> -4-Chlorophenylalanine               | 2.08(+1)  | 8.96(0) |        |        |
| 4-Chlorophenylarsonic acid                     | 3.33      | 8.25    |        |        |
| 2-Chlorophenylphosphonic acid                  | 1.63      | 6.98    |        |        |
| 3-Chlorophenylphosphonic acid                  | 1.55      | 6.65    |        |        |
| 4-Chlorophenylphosphonic acid                  | 1.66      | 6.75    |        |        |
| 3-(2'-Chlorophenyl)propanoic acid              | 4.577     |         |        |        |
| 3-(3'-Chlorophenyl)propanoic acid              | 4.585     |         |        |        |
| 3-(4'-Chlorophenyl)propanoic acid              | 4.607     |         |        |        |
| 3-Chlorophenylselenic acid                     | 4.47      |         |        |        |
| 4-Chlorophenylselenic acid                     | 4.48      |         |        |        |
| 4-Chloro-1,2-phthalic acid                     | 1.60      |         |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                          | $pK_1$    | $pK_2$    | $pK_3$ | $pK_4$ |
|----------------------------------------------------|-----------|-----------|--------|--------|
| 2-Chloropropanoic acid                             | 2.84      |           |        |        |
| 3-Chloropropanoic acid                             | 3.992     |           |        |        |
| 2-Chloropropylarsonic acid (18°C)                  | 3.76      | 8.39      |        |        |
| 3-Chloropropylarsonic acid (18°C)                  | 3.63      | 8.53      |        |        |
| Chloropropynoic acid                               | 1.854     |           |        |        |
| 2-Chloropyridine                                   | 0.49(+1)  |           |        |        |
| 3-Chloropyridine                                   | 2.84(+1)  |           |        |        |
| 4-Chloropyridine                                   | 3.83(+1)  |           |        |        |
| 7-Chlorotetracycline                               | 3.30(+1)  | 7.44      | 9.27   |        |
| 4-Chloro-2-(2'-thiazolylazo)phenol                 | 7.09      |           |        |        |
| 4-Chlorothiophenol                                 | 5.9       |           |        |        |
| <i>N</i> -Chloro- <i>p</i> -toluenesulfonamide     | 4.54(+1)  |           |        |        |
| 3-Chloro- <i>o</i> -toluidine                      | 2.49(+1)  |           |        |        |
| 4-Chloro- <i>o</i> -toluidine                      | 3.385(+1) |           |        |        |
| 5-Chloro- <i>o</i> -toluidine                      | 3.85(+1)  |           |        |        |
| 6-Chloro- <i>o</i> -toluidine                      | 3.62(+1)  |           |        |        |
| Chrome Azurol S                                    | 2.45      | 4.86      | 11.47  |        |
| Chrome Dark Blue                                   | 7.56      | 9.3       | 12.4   |        |
| Cinchonine                                         | 5.85(+2)  | 9.92(+1)  |        |        |
| <i>cis</i> -Cinnamic acid                          | 3.879     |           |        |        |
| <i>trans</i> -Cinnamic acid                        | 4.438     |           |        |        |
| Citraconic acid                                    | 2.29(0)   | 6.15(−1)  |        |        |
| Citric acid                                        | 3.128     | 4.761     | 6.396  |        |
| L-(+)-Citrulline                                   | 2.43(+1)  | 9.41(0)   |        |        |
| Cocaine                                            | 8.41(+1)  |           |        |        |
| Codeine                                            | 7.95(+1)  |           |        |        |
| Colchicine                                         | 1.65(+1)  |           |        |        |
| Coniine ( $\mu = 0.5$ )                            | 11.24(+1) |           |        |        |
| Creatine (40°C)                                    | 3.28(+1)  |           |        |        |
| Creatinine                                         | 3.57(+1)  |           |        |        |
| <i>o</i> -Cresol                                   | 10.26     |           |        |        |
| <i>m</i> -Cresol                                   | 10.00     |           |        |        |
| <i>p</i> -Cresol                                   | 10.26     |           |        |        |
| Cumene hydroperoxide                               | 12.60     |           |        |        |
| Cupreine                                           | 7.63(+1)  |           |        |        |
| Cyanamide                                          | 10.27     |           |        |        |
| Cyanoacetic acid                                   | 2.460     |           |        |        |
| Cyanoacetohydrazide                                | 2.34(+2)  | 11.17(+1) |        |        |
| 2-Cyanobenzoic acid                                | 3.14      |           |        |        |
| 3-Cyanobenzoic acid                                | 3.60      |           |        |        |
| 4-Cyanobenzoic acid                                | 3.55      |           |        |        |
| 4-Cyanobutanoic acid                               | 4.44      |           |        |        |
| <i>trans</i> -1-Cyanocyclohexane-2-carboxylic acid | 3.865     |           |        |        |
| 4-Cyano-2,6-dimethylphenol                         | 8.27      |           |        |        |
| 4-Cyano-3,5-dimethylphenol                         | 8.21      |           |        |        |
| 2-Cyanoethylamine                                  | 7.7(+1)   |           |        |        |
| <i>N</i> -(2-Cyano)ethylnorcodeine                 | 5.68(+1)  |           |        |        |
| Cyanomethylamine                                   | 5.34(+1)  |           |        |        |
| 2-Cyano-2-methyl-2-phenylacetic acid               | 2.290     |           |        |        |
| 1-Cyanomethylpiperidine                            | 4.55(+1)  |           |        |        |
| 2-Cyano-2-methylpropanoic acid                     | 2.422     |           |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                | $pK_1$    | $pK_2$   | $pK_3$   | $pK_4$ |
|----------------------------------------------------------|-----------|----------|----------|--------|
| 3-Cyanophenol                                            | 8.61      |          |          |        |
| <i>o</i> -Cyanophenoxyacetic acid                        | 2.98      |          |          |        |
| <i>m</i> -Cyanophenoxyacetic acid                        | 3.03      |          |          |        |
| <i>p</i> -Cyanophenoxyacetic acid                        | 2.93      |          |          |        |
| 2-Cyanopropanoic acid                                    | 2.37      |          |          |        |
| 3-Cyanopropanoic acid                                    | 3.99      |          |          |        |
| 2-Cyanopyridine                                          | -0.26(+1) |          |          |        |
| 3-Cyanopyridine                                          | 1.45(+1)  |          |          |        |
| 4-Cyanopyridine                                          | 1.90(+1)  |          |          |        |
| Cyanuric acid                                            | 6.78      |          |          |        |
| Cyclobutanecarboxylic acid                               | 4.785     |          |          |        |
| 1,1-Cyclobutanedicarboxylic acid                         | 3.13      | 5.88     |          |        |
| <i>cis</i> -1,2-Cyclobutanedicarboxylic acid             | 3.90      | 5.89     |          |        |
| <i>trans</i> -1,2-Cyclobutanedicarboxylic acid           | 3.79      | 5.61     |          |        |
| <i>cis</i> -1,3-Cyclobutanedicarboxylic acid             | 4.04      | 5.31     |          |        |
| <i>trans</i> -1,3-Cyclobutanedicarboxylic acid           | 3.81      | 5.28     |          |        |
| Cyclohexanecarboxylic acid                               | 4.90      |          |          |        |
| 1,1-Cyclohexanediactic acid                              | 3.49      | 6.96     |          |        |
| <i>cis</i> -1,2-Cyclohexanediactic acid (20°C)           | 4.42      | 5.45     |          |        |
| <i>trans</i> -1,2-Cyclohexanediactic acid (20°C)         | 4.38      | 5.42     |          |        |
| <i>cis</i> -1,2-Cyclohexanediamine                       | 6.43(+2)  | 9.93(+1) |          |        |
| <i>trans</i> -1,2-Cyclohexanediamine                     | 6.34(+2)  | 9.74(+1) |          |        |
| 1,1-Cyclohexanedicarboxylic acid                         | 3.45      | 4.11     |          |        |
| <i>cis</i> -1,2-Cyclohexanedicarboxylic acid (20°C)      | 4.34      | 6.76     |          |        |
| <i>trans</i> -1,2-Cyclohexanedicarboxylic acid (20°C)    | 4.18      | 5.93     |          |        |
| <i>cis</i> -1,3-Cyclohexanedicarboxylic acid (16°C)      | 4.10      | 5.46     |          |        |
| <i>trans</i> -1,3-Cyclohexanedicarboxylic acid (19°C)    | 4.31      | 5.73     |          |        |
| <i>trans</i> -1,4-Cyclohexanedicarboxylic acid (16°C)    | 4.18      | 5.42     |          |        |
| 1,3-Cyclohexanedione                                     | 5.26      |          |          |        |
| <i>cis,cis</i> -1,3,5-Cyclohexanetriamine                | 6.9(+3)   | 8.7(+2)  | 10.4(+1) |        |
| Cyclohexanimine                                          | 9.15      |          |          |        |
| <i>cis</i> -4-Cyclohexene-1,2-dicarboxylic acid (20°C)   | 3.89      | 6.79     |          |        |
| <i>trans</i> -4-Cyclohexene-1,2-dicarboxylic acid (20°C) | 3.95      | 5.81     |          |        |
| Cyclohexylacetic acid                                    | 4.51      |          |          |        |
| Cyclohexylamine                                          | 10.64(+1) |          |          |        |
| 2-(Cyclohexylamino)ethanesulfonic acid (CHES) (20°C)     | 9.55      |          |          |        |
| 3-Cyclohexylamino-1-propanesulfonic acid (CAPS) (20°C)   | 10.40     |          |          |        |
| 4-Cyclohexylbutanoic acid                                | 4.95      |          |          |        |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                                                  | $pK_1$       | $pK_2$   | $pK_3$    | $pK_4$      |
|----------------------------------------------------------------------------|--------------|----------|-----------|-------------|
| Cyclohexylcyanoacetic acid                                                 | 2.367        |          |           |             |
| 1,2-Cyclohexylenedinitriloacetic acid ( $\mu = 0.1$ )                      | 2.4          | 3.5      | 6.16      | 12.35       |
| 3-Cyclohexylpropanoic acid                                                 | 4.91         |          |           |             |
| 2-Cyclohexylpyrrolidine                                                    | 10.76(+1)    |          |           |             |
| 2-Cyclohexyl-2-pyrroline                                                   | 7.91(+1)     |          |           |             |
| Cyclohexylthioacetic acid                                                  | 3.488        |          |           |             |
| Cyclopentanecarboxylic acid                                                | 4.905        |          |           |             |
| cis-Cyclopentane-1-carboxylic acid-2-acetic acid                           | 4.40         | 5.79     |           |             |
| trans-Cyclopentane-1-carboxylic acid-2-acetic acid                         | 4.39         | 5.67     |           |             |
| Cyclopentane-1,2-diamine- <i>N,N',N'</i> -tetraacetic acid ( $\mu = 0.1$ ) | —            | —        | —         | 10.20       |
| Cyclopentane-1,1-dicarboxylic acid                                         | 3.23         | 4.08     |           |             |
| cis-Cyclopentane-1,2-dicarboxylic acid                                     | 4.43         | 6.67     |           |             |
| trans-Cyclopentane-1,2-dicarboxylic acid                                   | 3.96         | 5.85     |           |             |
| cis-Cyclopentane-1,3-dicarboxylic acid                                     | 4.26         | 5.51     |           |             |
| trans-Cyclopentane-1,3-dicarboxylic acid                                   | 4.32         | 5.42     |           |             |
| Cyclopentylamine                                                           | 10.65(+1)    |          |           |             |
| 1,1-Cyclopentylodiacetic acid                                              | 3.80         | 6.77     |           |             |
| cis-Cyclopentyl-1,2-diacetic acid                                          | 4.42         | 5.42     |           |             |
| trans-Cyclopentyl-1,2-diacetic acid                                        | 4.43         | 5.43     |           |             |
| Cyclopropanecarboxylic acid                                                | 4.827        |          |           |             |
| Cyclopropane-1,1-dicarboxylic acid                                         | 1.82         | 5.43     |           |             |
| cis-Cyclopropane-1,2-dicarboxylic acid                                     | 3.33         | 6.47     |           |             |
| trans-Cyclopropane-1,2-dicarboxylic acid                                   | 3.65         | 5.13     |           |             |
| Cyclopropylamine                                                           | 9.10(+1)     |          |           |             |
| 5-Cyclopropyl-1,2,3,4-tetrazole                                            | 4.90(+1)     |          |           |             |
| L-Cysteic acid (3-sulfo-L-alanine)                                         | 1.89(+1)     | 8.7(0)   |           |             |
| L-(+)-Cysteine                                                             | 1.96         | 8.18     | 10.29(SH) |             |
| L-(+)-Cysteine, ethyl ester                                                | 6.69         | 9.17(SH) |           |             |
|                                                                            | ( $NH_3^+$ ) |          |           |             |
| L-(+)-Cysteine, methyl ester                                               | 6.56         | 8.99(SH) |           |             |
|                                                                            | ( $NH_3^+$ ) |          |           |             |
| L-Cysteinyl-L-asparagine                                                   | 2.97         | 7.09     | 8.47      |             |
| L-Cystine (35°C)                                                           | 1.6(+2)      | 2.1(+1)  | 8.02(0)   | 8.71(−1)    |
| Cystinylglycylglycine (35°C)                                               | 3.12         | 3.21     | 6.01      | 6.87        |
| Cytidine                                                                   | 4.08(+1)     | 12.24(0) |           |             |
| Cytidine-2'-phosphoric acid                                                | 0.8(+1)      | 4.36(0)  | 6.17(−1)  |             |
| Cytidine-3'-phosphoric acid                                                | 0.80(+1)     | 4.31(0)  | 6.04(−1)  | 13.2(sugar) |
| Cytidine-5'-phosphoric acid                                                | —            | 4.39(0)  | 6.62(−1)  |             |
| Cytosine                                                                   | 4.58(+1)     | 12.15(0) |           |             |
| Decanedioic acid (sebacic acid)                                            | 4.59         | 5.59     |           |             |
| Dehydroascorbic acid (20°C)                                                | 3.21         | 7.92     | 10.3      |             |
| 2'-Deoxyadenosine ( $\mu = 0.1$ )                                          | 3.8(+1)      |          |           |             |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                              | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$    |
|------------------------------------------------------------------------|-----------|-----------|-----------|-----------|
| Deoxycholic acid                                                       | 6.58      |           |           |           |
| 2-Deoxyglucose                                                         | 12.52     |           |           |           |
| 2-Deoxyguanosine ( $\mu = 0.1$ )                                       | 2.5(+1)   |           |           |           |
| 5-Desoxypyridoxal ( $\mu = 0$ )                                        | 4.17(+1)  | 8.14(OH)  |           |           |
| 1,1-Diacetic acid semicarbazide<br>(30°C, $\mu = 0.1$ )                | 2.96      | 4.04      |           |           |
| Diacetylacetone                                                        | 7.42      |           |           |           |
| Diallylamine ( $\mu = 0.02$ )                                          | 9.29(+1)  |           |           |           |
| 5,5-Diallylbarbituric acid                                             | 7.78(0)   |           |           |           |
| 1,3-Diamino-2-aminomethylpropane                                       | 6.44(+3)  | 8.56(+2)  | 10.38(+1) |           |
| 3,5-Diaminobenzoic acid                                                | 5.30      |           |           |           |
| 1,3-Diamino- <i>N,N'</i> -bis-(2-aminoethyl)propane ( $\mu = 0.5$ )    | 6.01(+4)  | 7.26(+3)  | 9.49(+2)  | 10.23(+1) |
| 2,4-Diaminobutanoic acid (20°C)                                        | 1.85(+2)  | 8.24(+1)  | 10.40(0)  |           |
| 2,2'-Diaminodiethyl sulfide (30°C)                                     | 8.84(+2)  | 9.64(+1)  |           |           |
| 1,8-Diamino-3,6-dithiooctane<br>(30°C)                                 | 8.43(+2)  | 9.31(+1)  |           |           |
| 2,7-Diaminooctanedioic acid<br>(20°C, $\mu = 0.1$ )                    | 1.84(+2)  | 2.64(+1)  | 9.23(0)   | 9.89(-1)  |
| 1,8-Diamino-3,6-octanedione<br>(30°C)                                  | 8.60(+2)  | 9.57(+1)  |           |           |
| 1,8-Diamino-3-oxa-6-thiooctane                                         | 8.54(+2)  | 9.46(+1)  |           |           |
| 2,3-Diaminopropanoic acid ( $\mu = 0.1$ )                              | 1.33(+2)  | 6.674(+1) | 9.623(0)  |           |
| 2,3-Diaminopropanoic acid, methyl ester ( $\mu = 0.1$ )                | 4.412(+1) | 8.250(0)  |           |           |
| 1,3-Diamino-2-propanol (20°C)                                          | 7.93(+2)  | 9.69(+1)  |           |           |
| 2,5-Diaminopyridine (20°C)                                             | 2.13(+2)  | 6.48(+1)  |           |           |
| 1,4-Diazabicyclo[2.2.2]octane                                          | 2.90(+2)  | 8.60(+1)  |           |           |
| Dibenzylamine                                                          | 8.52(+1)  |           |           |           |
| Dibenzylsuccinic acid (20°C)                                           | 3.96      | 6.66      |           |           |
| Dibromoacetic acid                                                     | 1.39      |           |           |           |
| 3,5-Dibromoaniline                                                     | 2.35(+1)  |           |           |           |
| 3,5-Dibromophenol                                                      | 8.056     |           |           |           |
| 2,2-Dibromopropanoic acid                                              | 1.48      |           |           |           |
| 2,3-Dibromopropanoic acid                                              | 2.33      |           |           |           |
| <i>rac</i> -2,3-Dibromosuccinic acid<br>(20°C)                         | 1.43      | 2.24      |           |           |
| <i>meso</i> -2,3-Dibromosuccinic acid<br>(20°C)                        | 1.51      | 2.71      |           |           |
| 3,5-Dibromo- <i>p</i> -L-tyrosine                                      | 2.17(+1)  | 6.45(0)   | 7.60(-1)  |           |
| Dibutylamine                                                           | 11.25(+1) |           |           |           |
| Di- <i>sec</i> -butylamine                                             | 10.91(+1) |           |           |           |
| 2,6-Di- <i>tert</i> -butylpyridine                                     | 3.58(+1)  |           |           |           |
| <i>rac</i> -2,3-Di- <i>tert</i> -butylsuccinic acid<br>( $\mu = 0.1$ ) | 3.58      | 10.2      |           |           |
| 1,12-Dicarboxydodecaborane                                             | 9.07      | 10.23     |           |           |
| Dichloroacetic acid                                                    | 1.26      |           |           |           |
| Dichloroacetylacetic acid                                              | 2.11      |           |           |           |
| 3,5-Dichloroaniline                                                    | 2.37(+1)  |           |           |           |
| 1,3-Dichloro-2,5-dihydroxybenzene<br>( $\mu = 0.65$ )                  | 7.30      | 9.99      |           |           |



**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                            | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$   |
|------------------------------------------------------|-----------|-----------|-----------|----------|
| 2,5-Dichloro-3,6-dihydroxy- <i>p</i> -benzoquinone   | 1.09      | 2.42      |           |          |
| Dichloromethylphosphonic acid                        | 1.14      | 5.61      |           |          |
| 2,4-Dichloro-6-nitroaniline                          | -3.00(+1) |           |           |          |
| 2,5-Dichloro-4-nitroaniline                          | -1.74(+1) |           |           |          |
| 2,6-Dichloro-4-nitroaniline                          | -3.31(+1) |           |           |          |
| 2,3-Dichlorophenol                                   | 7.44      |           |           |          |
| 2,4-Dichlorophenol                                   | 7.85      |           |           |          |
| 2,6-Dichlorophenol                                   | 6.78      |           |           |          |
| 3,4-Dichlorophenol                                   | 8.630     |           |           |          |
| 3,5-Dichlorophenol                                   | 8.179     |           |           |          |
| 2,4-Dichlorophenoxyacetic acid (2,4-D)               | 2.64      |           |           |          |
| 4,6-Dichlorophenoxy-2-methylacetic acid              | 3.13      |           |           |          |
| 3,6-Dichlorophthalic acid                            | 1.46      |           |           |          |
| 2,2-Dichloropropanoic acid                           | 2.06      |           |           |          |
| 2,3-Dichloropropanoic acid                           | 2.85      |           |           |          |
| <i>rac</i> -2,3-Dichlorosuccinic acid (20°C)         | 1.43      | 2.81      |           |          |
| <i>meso</i> -2,3-Dichlorosuccinic acid               | 1.49      | 2.97      |           |          |
| 3,5-Dichloro- <i>p</i> -tyrosine                     | 2.12      | 6.47      | 7.62      |          |
| 2-Dicyanoethylamine                                  | 5.14(+1)  |           |           |          |
| 2,2-Dicyanopropanoic acid                            | -2.8      |           |           |          |
| Dicyclohexylamine                                    | 11.25(+1) |           |           |          |
| Dicyclopentylamine                                   | 10.93(+1) |           |           |          |
| Didodecylamine                                       | 10.99(+1) |           |           |          |
| Diethanolamine                                       | 8.88(+1)  |           |           |          |
| Di(ethoxyethyl)amine                                 | 8.47(+1)  |           |           |          |
| 3,5-Diethoxyphenol                                   | 9.370     |           |           |          |
| 3-(Diethoxyphosphinyl)benzoic acid                   | 3.65      |           |           |          |
| 4-(Diethoxyphosphinyl)benzoic acid                   | 3.60      |           |           |          |
| 3-(Diethoxyphosphinyl)phenol                         | 8.66      |           |           |          |
| 4-(Diethoxyphosphinyl)phenol                         | 8.28      |           |           |          |
| Diethylamine                                         | 10.8(+1)  |           |           |          |
| 2-(Diethylamino)ethyl-4-aminobenzoate                | 8.85(+1)  |           |           |          |
| $\alpha$ -(Diethylamino)toluene                      | 9.44(+1)  |           |           |          |
| <i>N,N</i> -Diethylaniline                           | 6.56(+1)  |           |           |          |
| 5,5-Diethylbarbituric acid (veronal)                 | 8.020(0)  |           |           |          |
| <i>N,N</i> -Diethylbenzylamine                       | 9.48(+1)  |           |           |          |
| Diethylbiguanide (30°C)                              | 2.53(+1)  | 11.68(0)  |           |          |
| Diethylenetriamine                                   | 4.42(+3)  | 9.21(+2)  | 10.02(+1) |          |
| Diethylenetriaminepentaacetic acid ( $pK_5$ , 10.58) | 1.80(0)   | 2.55(-1)  | 4.33(-2)  | 8.60(-3) |
| <i>N,N</i> -Diethylethylenediamine                   | 7.70(+2)  | 10.46(+1) |           |          |
| 2,2-Diethylglutaric acid                             | 3.62      | 7.12      |           |          |
| <i>N,N</i> -Diethylglycine                           | 2.04(+1)  | 10.47(0)  |           |          |
| Diethylglycolic acid (18°C)                          | 3.804     |           |           |          |
| Diethylmalonic acid                                  | 2.151     | 7.417     |           |          |
| Diethylmethylamine                                   | 10.43(+1) |           |           |          |
| <i>rac</i> -2,3-Diethylsuccinic acid                 | 3.63      | 6.46      |           |          |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                             | $pK_1$   | $pK_2$    | $pK_3$    | $pK_4$   |
|-----------------------------------------------------------------------|----------|-----------|-----------|----------|
| <i>meso</i> -2,3-Diethylsuccinic acid                                 | 3.54     | 6.59      |           |          |
| <i>N,N</i> -Diethyl- <i>o</i> -toluidine                              | 7.18(+1) |           |           |          |
| Difluoroacetic acid                                                   | 1.33     |           |           |          |
| 3,3-Difluoroacrylic acid                                              | 3.17     |           |           |          |
| Diglycolic acid                                                       | 2.96     |           |           |          |
| Diguanidine                                                           | 12.8     |           |           |          |
| Dihexylamine                                                          | 11.0(+1) |           |           |          |
| Dihydroarecaidine                                                     | 9.70     |           |           |          |
| Dihydroarecaidine, methyl ester                                       | 8.39     |           |           |          |
| Dihydrocodeine                                                        | 8.75(+1) |           |           |          |
| Dihydroergonovine                                                     | 7.38(+1) |           |           |          |
| $\alpha$ -Dihydrolysergic acid                                        | 3.57     | 8.45      |           |          |
| $\gamma$ -Dihydrolysergic acid                                        | 3.60     | 8.71      |           |          |
| $\alpha$ -Dihydrolysergol                                             | 8.30     |           |           |          |
| $\beta$ -Dihydrolysergol                                              | 8.23     |           |           |          |
| Dihydromorphine                                                       | 9.35     |           |           |          |
| 3,4-Dihydroxyalanine                                                  | 2.32(+1) | 8.68(0)   | 9.87(-1)  |          |
| 1,2-Dihydroxyanthraquinone-3-sulfonic acid (alizarin-3-sulfonic acid) | —        | 5.54(-1)  | 11.01(-2) |          |
| 3,4-Dihydroxybenzaldehyde                                             | 7.55     |           |           |          |
| 1,2-Dihydroxybenzene (pyrocatechol) ( $\mu = 0.1$ )                   | 9.356(0) | 12.98(-1) |           |          |
| 1,3-Dihydroxybenzene (resorcinol)                                     | 9.44(0)  | 12.32(-1) |           |          |
| 1,4-Dihydroxybenzene (hydroquinone)                                   | 9.91(0)  | 12.04(-1) |           |          |
| 4,5-Dihydroxybenzene-1,3-disulfonic acid                              | —        | —         | 7.66(-2)  | 12.6(-3) |
| 2,3-Dihydroxybenzoic acid (30°C)                                      | 2.98     | 10.14     |           |          |
| 2,4-Dihydroxybenzoic acid ( $\beta$ -resorcylic acid)                 | 3.29     | 8.98      |           |          |
| 2,5-Dihydroxybenzoic acid                                             | 2.97     | 10.50     |           |          |
| 2,6-Dihydroxybenzoic acid                                             | 1.30     |           |           |          |
| 3,4-Dihydroxybenzoic acid                                             | 4.48     | 8.67      | 11.74     |          |
| 3,5-Dihydroxybenzoic acid                                             | 4.04     |           |           |          |
| 2,5-Dihydroxy- <i>p</i> -benzoquinone                                 | 2.71     | 5.18      |           |          |
| 3,4-Dihydroxy-3-cyclobutene-1,2-dione                                 | 0.541    | 3.480     |           |          |
| 2,3-Dihydroxy-2-cyclopenten-1-one (20°C)                              | 4.72     |           |           |          |
| 1,4-Dihydroxy-2,6-dinitrobenzene                                      | 4.42     | 9.14      |           |          |
| Di(2,2'-hydroxyethyl)amine                                            | 8.8(+1)  |           |           |          |
| <i>N,N</i> -Di(2-hydroxyethyl)glycine                                 | 8.333    |           |           |          |
| Dihydroxymaleic acid                                                  | 1.10     |           |           |          |
| Dihydroxymalic acid                                                   | 1.92     |           |           |          |
| 1,3-Dihydroxy-2-methylbenzene ( $\mu = 0.65$ )                        | 10.05    | 11.64     |           |          |
| 2,2-Di(hydroxymethyl)-3-hydroxypropanoic acid                         | 4.460    |           |           |          |
| 2,4-Dihydroxy-5-methylpyrimidine                                      | 9.90     |           |           |          |
| 2,4-Dihydroxy-6-methylpyrimidine                                      | 9.52     |           |           |          |
| 1,4-Dihydroxynaphthalene (26°C, $\mu = 0.65$ )                        | 9.37     | 10.93     |           |          |
| 1,2-Dihydroxy-3-nitrobenzene                                          | 6.68     |           |           |          |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                                      | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$    |
|----------------------------------------------------------------|-----------|-----------|-----------|-----------|
| 1,2-Dihydroxy-4-nitrobenzene<br>( $\mu = 0.1$ )                | 6.701     |           |           |           |
| 2,4-Dihydroxy-1-phenylazobenzene<br>( $\mu = 0.1$ )            | 11.98     |           |           |           |
| 2,4-Dihydroxyoxazolidine                                       | 6.11(+1)  |           |           |           |
| 2,4-Dihydroxypteridine                                         | <1.3      | 7.92      |           |           |
| 2,6-Dihydroxypurine                                            | 7.53(0)   | 11.84(−1) |           |           |
| 2,4-Dihydroxypyridine (20°C)                                   | 1.37(+1)  | 6.45(0)   | 13(−1)    |           |
| Dihydroxytartaric acid                                         | 1.95      | 4.00      |           |           |
| 1,4-Dihydroxy-2,3,5,6-tetramethyl-<br>benzene ( $\mu = 0.65$ ) | 11.25     | 12.70     |           |           |
| 3,5-Diiodoaniline                                              | 2.37(+1)  |           |           |           |
| 2,5-Diiodohistamine                                            | 2.31(+2)  | 8.20(+1)  | 10.11(0)  |           |
| 2,5-Diiodohistidine ( $\mu = 0.1$ )                            | 2.72      | 8.18      | 9.76      |           |
| 3,5-Diiodophenol                                               | 8.103     |           |           |           |
| 3,5-Diiodotyrosine                                             | 2.117(+1) | 6.479(0)  | 7.821(−1) |           |
| Diisopropylmalonic acid                                        | 2.124     | 8.848     |           |           |
| Dilactic acid                                                  | 2.955     |           |           |           |
| <i>threo</i> -1,4-Dimercapto-2,3-butane-<br>diol               | 8.9       |           |           |           |
| <i>meso</i> -2,3-Dimercaptosuccinic acid                       | 2.71      | 3.48      | 8.89(SH)  | 10.79(SH) |
| 3,5-Dimethoxyaniline                                           | 3.86(+1)  |           |           |           |
| 2,6-Dimethoxybenzoic acid                                      | 3.44      |           |           |           |
| 1,10-Dimethoxy-3,8-dimethyl-4,7-<br>phenanthroline             | 7.21      |           |           |           |
| Di(2-methoxyethyl)amine                                        | 9.51(+1)  |           |           |           |
| 3,5-Dimethoxyphenol                                            | 9.345     |           |           |           |
| (3,4-Dimethoxy)phenylacetic acid                               | 4.333     |           |           |           |
| Dimethylamine                                                  | 10.77(+1) |           |           |           |
| 4-Dimethylaminobenzaldehyde                                    | 1.647(+1) |           |           |           |
| <i>N,N</i> -Dimethylaminocyclohexane                           | 10.72(+1) |           |           |           |
| 4-Dimethylamino-2,3-dimethyl-1-<br>phenyl-3-pyrazolin-5-one    | 4.18(+1)  |           |           |           |
| 4-Dimethylamino-3,5-dimethylpyr-<br>idine (20°C)               | 8.15(+1)  |           |           |           |
| 2-(Dimethylamino)ethanol                                       | 9.26(+1)  |           |           |           |
| 2-[2-(Dimethyl-<br>amino)ethyl]pyridine                        | 3.46(+2)  | 8.75(+1)  |           |           |
| 3-(Dimethylaminoethyl)pyridine                                 | 4.30(+2)  | 8.86(+1)  |           |           |
| 4-(Dimethylaminoethyl)pyridine                                 | 4.66(+2)  | 8.70(+1)  |           |           |
| 4-(Dimethylamino)-3-ethylpyridine<br>(20°C)                    | 8.66(+1)  |           |           |           |
| 4-(Dimethylamino)-3-isopropylpyr-<br>idine (20°C)              | 8.27(+1)  |           |           |           |
| 2-(Dimethylaminomethyl)pyridine                                | 2.58(+2)  | 8.12(+1)  |           |           |
| 3-(Dimethylaminomethyl)pyridine                                | 3.17(+2)  | 8.00(+1)  |           |           |
| 4-(Dimethylaminomethyl)pyridine                                | 3.39(+2)  | 7.66(+1)  |           |           |
| 4-(Dimethylamino)-3-methylpyri-<br>dine (20°C)                 | 8.68(+1)  |           |           |           |
| 4-(Dimethylamino-<br>phenyl)phosphonic acid                    | 2.0(+1)   | 4.2       | 7.35      |           |
| 3-(Dimethylamino)propanoic acid                                | 9.85(+1)  |           |           |           |
| 4-(Dimethylamino)pyridine (20°C)                               | 6.09(+1)  |           |           |           |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                        | $pK_1$                  | $pK_2$    | $pK_3$ | $pK_4$ |
|------------------------------------------------------------------|-------------------------|-----------|--------|--------|
| <i>N,N</i> -Dimethylaniline                                      | 5.15(+1)                |           |        |        |
| 2,3-Dimethylaniline                                              | 4.70(+1)                |           |        |        |
| 2,4-Dimethylaniline                                              | 4.89(+1)                |           |        |        |
| 2,5-Dimethylaniline                                              | 4.53(+1)                |           |        |        |
| 2,6-Dimethylaniline                                              | 3.95(+1)                |           |        |        |
| 3,4-Dimethylaniline                                              | 5.17(+1)                |           |        |        |
| 3,5-Dimethylaniline                                              | 4.765(+1)               |           |        |        |
| <i>N,N</i> -Dimethylaniline-4-phosphonic acid (17°C)             | 2.0(+1)                 | 4.2       | 7.39   |        |
| Dimethylarsinic acid (cacodylic acid)                            | 1.67                    | 6.273     |        |        |
| 1,3-Dimethylbarbituric acid                                      | 4.68(+1)                |           |        |        |
| 2,3-Dimethylbenzoic acid                                         | 3.771                   |           |        |        |
| 2,4-Dimethylbenzoic acid                                         | 4.217                   |           |        |        |
| 2,5-Dimethylbenzoic acid                                         | 3.990                   |           |        |        |
| 2,6-Dimethylbenzoic acid                                         | 3.362                   |           |        |        |
| 3,4-Dimethylbenzoic acid                                         | 4.41                    |           |        |        |
| 3,5-Dimethylbenzoic acid                                         | 4.302                   |           |        |        |
| <i>N,N</i> -Dimethylbenzylamine                                  | 9.02(+1)                |           |        |        |
| Dimethylbiguanide                                                | 2.77(+1)                | 11.52     |        |        |
| 2,2-Dimethylbutanoic acid (18°C)                                 | 5.03                    |           |        |        |
| Dimethylchlorotetracycline ( $\mu = 0.01$ )                      | 3.30(+1)                |           |        |        |
| 2,6-Dimethyl-4-cyanophenol                                       | 8.27                    |           |        |        |
| 3,5-Dimethyl-4-cyanophenol                                       | 8.21                    |           |        |        |
| 5,5-Dimethyl-1,3-cyclohexanedione                                | 5.15                    |           |        |        |
| <i>cis</i> -3,3-Dimethyl-1,2-cyclopropane-dicarboxylic acid      | 2.34                    | 8.31      |        |        |
| <i>trans</i> -3,3-Dimethyl-1,2-cyclopropanedicarboxylic acid     | 3.92                    | 5.32      |        |        |
| 3,5-Dimethyl-4-(dimethylamino)-pyridine (20°C)                   | 8.12(+1)                |           |        |        |
| 2,2-Dimethyl-1,3-dioxane-4,6-dione                               | 5.1                     |           |        |        |
| 1,1-Dimethylethanethiol ( $\mu = 0.1$ )                          | 11.22                   |           |        |        |
| <i>N,N</i> -Dimethylethylenediamine- <i>N,N</i> -diacetic acid   | 6.63                    | 9.53      |        |        |
| <i>N,N'</i> -Dimethylethylenediamine- <i>N,N'</i> -diacetic acid | 7.40                    | 10.16     |        |        |
| <i>N,N</i> -Dimethylethylenediamine- <i>N,N'</i> -diacetic acid  | 5.99                    | 9.97      |        |        |
| <i>N,N</i> -Dimethylglycine                                      | 2.146(+1)               | 9.940(0)  |        |        |
| Dimethylglycolic acid (18°C)                                     | 4.04                    |           |        |        |
| <i>N,N</i> -Dimethylglycylglycine                                | 3.11(+1)                | 8.09(0)   |        |        |
| Dimethylglyoxime                                                 | 10.60                   |           |        |        |
| 5,5-Dimethyl-2,4-hexanedione                                     | 10.01                   |           |        |        |
| 5,5-Dimethylhydantoin                                            | 9.19                    |           |        |        |
| 2,4-Dimethyl-8-hydroxyquinoline                                  | 6.20(+1)                | 10.60(0)  |        |        |
| 3,4-Dimethyl-8-hydroxyquinoline                                  | 5.80(+1)                | 10.05(0)  |        |        |
| 2,4-Dimethyl-8-hydroxyquinoline-7-sulfonic acid                  | 3.20 (NH <sup>+</sup> ) | 10.14(OH) |        |        |
| Dimethylhydroxytetracycline                                      | 7.5                     | 9.4       |        |        |
| 2,4-Dimethylimidazole                                            | 8.38(+1)                |           |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                         | $pK_1$    | $pK_2$    | $pK_3$ | $pK_4$ |
|---------------------------------------------------|-----------|-----------|--------|--------|
| Dimethylmalic acid                                | 3.17      | 6.06      |        |        |
| 2,2-Dimethylmalonic acid                          | 3.17      | 6.06      |        |        |
| 3,5-Dimethyl-4-(methylamino) pyr-<br>idine (20°C) | 9.96(+1)  |           |        |        |
| 2,3-Dimethylnaphthalene-1-carbox-<br>ylic acid    | 3.33      |           |        |        |
| 2,6-Dimethyl-4-nitrophenol                        | 7.190     |           |        |        |
| 3,5-Dimethyl-4-nitrophenol                        | 8.245     |           |        |        |
| $\alpha,\alpha$ -Dimethyloxaloacetic acid         | 1.77      | 4.62      |        |        |
| 3,3-Dimethylpentanedioic acid                     | 3.70      | 6.34      |        |        |
| 2,2-Dimethylpentanoic acid                        | 4.969     |           |        |        |
| 4,4-Dimethylpentanoic acid (18°C)                 | 4.79      |           |        |        |
| 2,3-Dimethylphenol                                | 10.50     |           |        |        |
| 2,4-Dimethylphenol                                | 10.58     |           |        |        |
| 2,5-Dimethylphenol                                | 10.22     |           |        |        |
| 2,6-Dimethylphenol                                | 10.59     |           |        |        |
| 3,4-Dimethylphenol                                | 10.32     |           |        |        |
| 3,5-Dimethylphenol                                | 10.15     |           |        |        |
| 2,6-Dimethylphenoxyacetic acid                    | 3.356     |           |        |        |
| Dimethylphenylsilylacetic acid                    | 5.27      |           |        |        |
| <i>N,N'</i> -Dimethylpiperazine                   | 4.630(+2) | 8.539(+1) |        |        |
| 1,2-Dimethylpiperidine                            | 10.22     |           |        |        |
| <i>cis</i> -2,6-Dimethylpiperidine                | 11.07(+1) |           |        |        |
| 2,2-Dimethylpropanoic acid (pi-<br>valic acid)    | 5.031     |           |        |        |
| 2,2'-Dimethylpropylphosphonic<br>acid             | 2.84      | 8.65      |        |        |
| 2,4-Dimethylpyridine (2,4-lutidine)               | 6.74(+1)  |           |        |        |
| 2,5-Dimethylpyridine (2,5-lutidine)               | 6.43(+1)  |           |        |        |
| 2,6-Dimethylpyridine (2,6-lutidine)               | 6.71(+1)  |           |        |        |
| 3,4-Dimethylpyridine (3,4-lutidine)               | 6.47(+1)  |           |        |        |
| 3,5-Dimethylpyridine (3,5-lutidine)               | 6.09(+1)  |           |        |        |
| 2,4-Dimethylpyridine-1-oxide                      | 1.627(+1) |           |        |        |
| 2,5-Dimethylpyridine-1-oxide                      | 1.208(+1) |           |        |        |
| 2,6-Dimethylpyridine-1-oxide                      | 1.366(+1) |           |        |        |
| 3,4-Dimethylpyridine-1-oxide                      | 1.493(+1) |           |        |        |
| 3,5-Dimethylpyridine-1-oxide                      | 1.181(+1) |           |        |        |
| 2,3-Dimethylquinoline                             | 4.94(+1)  |           |        |        |
| 2,6-Dimethylquinoline                             | 5.46(+1)  |           |        |        |
| <i>meso</i> -2,2-Dimethylsuccinic acid            | 3.77      | 5.936     |        |        |
| <i>rac</i> -2,2-Dimethylsuccinic acid             | 3.93      | 6.20      |        |        |
| <b>D</b> -2,3-Dimethylsuccinic acid               | 3.82      | 5.93      |        |        |
| <i>meso</i> -2,3-Dimethylsuccinic acid            | 3.67      | 5.30      |        |        |
| <i>rac</i> -2,3-Dimethylsuccinic acid             | 3.94      | 6.20      |        |        |
| 2,4-Dimethylthiazole ( $\mu = 0.1$ )              | 3.98      |           |        |        |
| 2,5-Dimethylthiazole ( $\mu = 0.1$ )              | 3.91      |           |        |        |
| 4,5-Dimethylthiazole ( $\mu = 0.1$ )              | 3.73      |           |        |        |
| <i>N,N</i> -Dimethyl- <i>o</i> -toluidine         | 5.86(+1)  |           |        |        |
| <i>N,N</i> -Dimethyl- <i>p</i> -toluidine         | 7.24(+1)  |           |        |        |
| 2,4-Dinitroaniline                                | -4.25(+1) |           |        |        |
| 2,6-Dinitroaniline                                | -5.23(+1) |           |        |        |
| 3,5-Dinitroaniline                                | 0.229(+1) |           |        |        |
| 2,3-Dinitrobenzoic acid                           | 1.85      |           |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                      | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$ |
|--------------------------------------------------------------------------------|-----------|-----------|-----------|--------|
| 2,4-Dinitrobenzoic acid                                                        | 1.43      |           |           |        |
| 2,5-Dinitrobenzoic acid                                                        | 1.62      |           |           |        |
| 2,6-Dinitrobenzoic acid                                                        | 1.14      |           |           |        |
| 3,4-Dinitrobenzoic acid                                                        | 2.82      |           |           |        |
| 3,5-Dinitrobenzoic acid                                                        | 2.85      |           |           |        |
| 1,1-Dinitrobutane (20°C)                                                       | 5.90      |           |           |        |
| 1,1-Dinitrodecane                                                              | 3.60      |           |           |        |
| 1,1-Dinitroethane (20°C)                                                       | 5.21      |           |           |        |
| Dinitromethane (20°C)                                                          | 3.60      |           |           |        |
| 1,1-Dinitropentane                                                             | 5.337     |           |           |        |
| 2,4-Dinitrophenol                                                              | 4.08      |           |           |        |
| 2,5-Dinitrophenol                                                              | 5.216     |           |           |        |
| 2,6-Dinitrophenol                                                              | 3.713     |           |           |        |
| 3,4-Dinitrophenol                                                              | 5.424     |           |           |        |
| 3,5-Dinitrophenol                                                              | 6.732     |           |           |        |
| 2,4-Dinitrophenylacetic acid                                                   | 3.50      |           |           |        |
| 1,1-Dinitropropane (20°C)                                                      | 5.5       |           |           |        |
| 2,6-Dioxo-1,2,3,6-tetrahydro-4-pyr-<br>imidinecarboxylic acid (orotic<br>acid) | 1.8(+1)   | 9.55(0)   |           |        |
| Diphenylacetic acid                                                            | 3.939     |           |           |        |
| Diphenylamine                                                                  | 0.9(+1)   |           |           |        |
| 2,2-Diphenylglutaric acid (20°C)                                               | 3.91      | 5.38      |           |        |
| 1,3-Diphenylguanidine                                                          | 10.12     |           |           |        |
| 2,2-Diphenylheptanedioic acid<br>(20°C)                                        | 4.28      | 5.39      |           |        |
| 2,2-Diphenylhexanedioic acid<br>(20°C)                                         | 4.17      | 5.40      |           |        |
| 3,3-Diphenylhexanedioic acid                                                   | 4.22      | 5.19      |           |        |
| Diphenylhydroxyacetic acid<br>(35°C)                                           | 3.05      |           |           |        |
| Diphenylketimine                                                               | 6.82      |           |           |        |
| 2,2-Diphenylnonanedioic acid<br>(20°C)                                         | 4.33      | 5.38      |           |        |
| <i>meso</i> -2,2-Diphenylsuccinic acid                                         | 3.48      |           |           |        |
| <i>rac</i> -2,2-Diphenylsuccinic acid                                          | 3.58      |           |           |        |
| 2,2-Diphenylsuccinic acid, 1-<br>methyl ester (20°C)                           | 4.47      |           |           |        |
| 2,2-Diphenylsuccinic acid, 4-<br>methyl ester (20°C)                           | 3.900     |           |           |        |
| Diphenylthiocarbazone                                                          | 4.50      | 15        |           |        |
| Dipropylamine                                                                  | 10.91(+1) |           |           |        |
| Dipropyleneetriamine                                                           | 7.72(+3)  | 9.56(+2)  | 10.65(+1) |        |
| 2,2-Dipropylglutaric acid                                                      | 3.688     | 7.31      |           |        |
| Dipropylmalonic acid                                                           | 2.04      | 7.51      |           |        |
| 2,2'-Dipyridyl                                                                 | -0.52(+2) | 4.352(+1) |           |        |
| 2,3'-Dipyridyl (20°C)                                                          | 1.52(+2)  | 4.42(+1)  |           |        |
| 2,4'-Dipyridyl (20°C)                                                          | 1.19(+2)  | 4.77(+1)  |           |        |
| 3,3'-Dipyridyl (20°C, $\mu = 0.2$ )                                            | 3.0(+2)   | 4.60(+1)  |           |        |
| 3,4'-Dipyridyl (20°C, $\mu = 0.2$ )                                            | 3.0(+2)   | 4.85(+1)  |           |        |
| 4,4'-Dipyridyl                                                                 | 3.17(+2)  | 4.82(+1)  |           |        |
| Dithiodiacetic acid (18°C)                                                     | 3.075     | 4.201     |           |        |
| 1,4-Dithioerythritol                                                           | 9.5       |           |           |        |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                                                    | $pK_1$    | $pK_2$     | $pK_3$   | $pK_4$ |
|------------------------------------------------------------------------------|-----------|------------|----------|--------|
| Dithiooxamide (rubeanic acid)                                                | 10.89     |            |          |        |
| Dulcitol                                                                     | 13.46     |            |          |        |
| Ecgonine                                                                     | 10.91     |            |          |        |
| Emetine                                                                      | 7.36(+1)  | 8.23(0)    |          |        |
| Epinephrine enantiomorph                                                     | 9.39(+1)  |            |          |        |
| Epinephrine, pseudo                                                          | 9.53(+1)  |            |          |        |
| Ergometrinine                                                                | 7.32(+1)  |            |          |        |
| Ergonovine                                                                   | 6.73(+1)  |            |          |        |
| Eriochrome Black T                                                           | 6.3       | 11.55      |          |        |
| 1,2-Ethanediamine                                                            | 6.85(+2)  | 9.92(+1)   |          |        |
| Ethane-1,2-diamino- <i>N,N'</i> -dimethyl- <i>N,N'</i> -diacetic acid (20°C) | 6.047(0)  | 10.068(−1) |          |        |
| 1,2-Ethanedithiol                                                            | 8.96      | 10.54      |          |        |
| Ethanethiol ( $\mu = 0.015$ )                                                | 10.61     |            |          |        |
| Ethoxyacetic acid (18°C)                                                     | 3.65      |            |          |        |
| 2-Ethoxyaniline ( <i>o</i> -phenetidine)                                     | 4.47(+1)  |            |          |        |
| 3-Ethoxyaniline                                                              | 4.17(+1)  |            |          |        |
| 4-Ethoxyaniline                                                              | 5.25(+1)  |            |          |        |
| 2-Ethoxybenzoic acid (20°C)                                                  | 4.21      |            |          |        |
| 3-Ethoxybenzoic acid (20°C)                                                  | 4.17      |            |          |        |
| 4-Ethoxybenzoic acid (20°C)                                                  | 4.80      |            |          |        |
| Ethoxycarbonylethylamine                                                     | 9.13(+1)  |            |          |        |
| 2-Ethoxyethanethiol                                                          | 9.38      |            |          |        |
| 2-Ethoxyethylamine                                                           | 6.26(+1)  |            |          |        |
| 2-Ethoxyphenol                                                               | 10.109    |            |          |        |
| 3-Ethoxyphenol                                                               | 9.655     |            |          |        |
| (4-Ethoxyphenyl)phosphonic acid                                              | 2.06      | 7.28       |          |        |
| 4-Ethoxypyridine                                                             | 6.67(+1)  |            |          |        |
| Ethyl acetoacetate                                                           | 10.68     |            |          |        |
| 3-Ethylacrylic acid                                                          | 4.695     |            |          |        |
| <i>N</i> -Ethylalanine                                                       | 2.22(+1)  | 10.22(0)   |          |        |
| Ethylamine                                                                   | 10.63(+1) |            |          |        |
| (3-Ethylamino)phenylphosphonic acid                                          | 1.1(+1)   | 4.90(0)    | 7.24(−1) |        |
| <i>N</i> -Ethylaniline                                                       | 5.11(+1)  |            |          |        |
| 2-Ethylaniline                                                               | 4.42(+1)  |            |          |        |
| 3-Ethylaniline                                                               | 4.70(+1)  |            |          |        |
| 4-Ethylaniline                                                               | 5.00(+1)  |            |          |        |
| Ethylarsonic acid (18°C)                                                     | 3.89      | 8.35       |          |        |
| Ethylbarbituric acid                                                         | 3.69(+1)  |            |          |        |
| 2-Ethylbenzimidazole ( $\mu = 0.16$ )                                        | 6.27(+1)  |            |          |        |
| 2-Ethylbenzoic acid                                                          | 3.79      |            |          |        |
| 4-Ethylbenzoic acid                                                          | 4.35      |            |          |        |
| Ethylbiguanide                                                               | 2.09(+1)  | 11.47(0)   |          |        |
| 2-Ethylbutanoic acid (20°C)                                                  | 4.710     |            |          |        |
| <i>S</i> -Ethyl- <i>L</i> -cysteine ( $\mu = 0.1$ )                          | 2.03(+1)  | 8.60(0)    |          |        |
| Ethylenebiguanide (30°C)                                                     | 1.74      | 2.88       | 11.34    | 11.76  |
| Ethylenebis(thioacetic acid) (18°C)                                          | 3.382(0)  | 4.352(−1)  |          |        |
| Ethylenediamine- <i>N,N'</i> -diacetic acid                                  | 6.42      | 9.46       |          |        |
| Ethylenediamine- <i>N,N</i> -dimethyl- <i>N',N'</i> -diacetic acid           | 6.047     | 10.068     |          |        |
| Ethylenediamine- <i>N,N</i> -dipropanoic acid (30°C)                         | 6.87      | 9.60       |          |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                            | $pK_1$     | $pK_2$    | $pK_3$ | $pK_4$ |
|----------------------------------------------------------------------|------------|-----------|--------|--------|
| Ethylenediamine- <i>N,N,N',N'</i> -tetra-acetic acid ( $\mu = 0.1$ ) | 1.99       | 2.67      | 6.16   | 10.26  |
| Ethylenediamine- <i>N,N,N',N'</i> -tetra-propanoic acid (30°C)       | 3.00       | 3.43      | 6.77   | 9.60   |
| Ethylene glycol                                                      | 14.22      |           |        |        |
| Ethyleneimine                                                        | 8.04(+1)   |           |        |        |
| <i>cis</i> -Ethylene oxide dicarboxylic acid                         | 1.93       | 3.92      |        |        |
| <i>trans</i> -Ethylene oxide dicarboxylic acid                       | 1.93       | 3.25      |        |        |
| <i>N</i> -Ethylethylenediamine                                       | 7.63(+2)   | 10.56(+1) |        |        |
| <i>N</i> -Ethylglycine ( $\mu = 0.1$ )                               | 2.34(+1)   | 10.23(0)  |        |        |
| 3-Ethylglutaric acid                                                 | 4.28       | 5.33      |        |        |
| Ethyl hydroperoxide                                                  | 11.80      |           |        |        |
| Ethyl hydrogen malonate                                              | 3.55       |           |        |        |
| 3-Ethyl-2-hydroxypyridine                                            | 5.00(+1)   |           |        |        |
| Ethylmalonic acid                                                    | 2.90(0)    | 5.55(−1)  |        |        |
| <i>N</i> -Ethyl mercaptoacetamide                                    | 8.14(SH)   |           |        |        |
| Ethyl 2-mercaptoacetate                                              | 7.95(SH)   |           |        |        |
| Ethyl 3-mercaptopropanoate                                           | 9.48(SH)   |           |        |        |
| 3-Ethyl-4-(methylamino)pyridine (20°C)                               | 9.90(+1)   |           |        |        |
| 5-Ethyl-5-(1-methylbutyl)barbituric acid                             | 8.11(0)    |           |        |        |
| Ethyl methyl ketoxime                                                | 12.45      |           |        |        |
| Ethylmethylmalonic acid                                              | 2.86(0)    | 6.41(−1)  |        |        |
| 1-Ethyl-2-methylpiperidine                                           | 10.66(+1)  |           |        |        |
| 3-Ethyl-6-methylpyridine (20°C)                                      | 6.51(+1)   |           |        |        |
| 3-Ethyl-4-methylpyridine-1-oxide                                     | −1.534(+1) |           |        |        |
| 5-Ethyl-2-methylpyridine-1-oxide                                     | −1.288(+1) |           |        |        |
| 1-Ethyl-2-methyl-2-pyrroline                                         | 11.84(+1)  |           |        |        |
| Ethylmorphine (15°C)                                                 | 8.08       |           |        |        |
| Ethyl nitroacetate                                                   | 5.85       |           |        |        |
| 3-Ethylpentane-2,4-dione                                             | 11.34      |           |        |        |
| 2-Ethylpentanoic acid (18°C)                                         | 4.71       |           |        |        |
| 5-Ethyl-5-pentylbarbituric acid                                      | 7.960      |           |        |        |
| 2-Ethylphenol                                                        | 10.2       |           |        |        |
| 3-Ethylphenol                                                        | 10.07      |           |        |        |
| 4-Ethylphenol                                                        | 10.0       |           |        |        |
| 4-Ethylphenylacetic acid                                             | 4.373      |           |        |        |
| 5-Ethyl-5-phenylbarbituric acid                                      | 7.445      |           |        |        |
| Ethylphosphinic acid                                                 | 3.29       |           |        |        |
| Ethylphosphonic acid                                                 | 2.43       | 8.05      |        |        |
| 1-Ethylpiperidine ( $\mu = 0.01$ )                                   | 10.45(+1)  |           |        |        |
| 2,2-Ethylpropylglutaric acid                                         | 3.511      |           |        |        |
| Ethylpropylmalonic acid                                              | 3.14       | 7.43      |        |        |
| 2-Ethylpyridine                                                      | 5.89(+1)   |           |        |        |
| 3-Ethylpyridine (20°C)                                               | 5.80(+1)   |           |        |        |
| 4-Ethylpyridine                                                      | 5.87(+1)   |           |        |        |
| Ethyl 3-pyridinecarboxylate                                          | 3.35(+1)   |           |        |        |
| Ethyl 4-pyridinecarboxylate                                          | 3.45(+1)   |           |        |        |
| 2-Ethylpyridine-1-oxide                                              | −1.19(+1)  |           |        |        |
| 3-Ethylpyridine-1-oxide                                              | −0.965(+1) |           |        |        |
| Ethylpyrrolidine                                                     | 10.43(+1)  |           |        |        |



**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                              | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$ |
|----------------------------------------|-----------|-----------|-----------|--------|
| 2-Ethyl-2-pyrroline                    | 7.87(+1)  |           |           |        |
| Ethylsuccinic acid                     | 4.08(0)   |           |           |        |
| S-Ethylthioacetic acid                 | 5.06      |           |           |        |
| N-Ethyl- <i>o</i> -toluidine           | 4.92(+1)  |           |           |        |
| N-Ethylveratramine                     | 7.40(+1)  |           |           |        |
| $\beta$ -Eucaine                       | 9.35(+1)  |           |           |        |
| Fluoroacetic acid                      | 2.586     |           |           |        |
| 2-Fluoroacrylic acid                   | 2.55      |           |           |        |
| 2-Fluoroaniline                        | 3.20(+1)  |           |           |        |
| 3-Fluoroaniline                        | 3.58(+1)  |           |           |        |
| 4-Fluoroaniline                        | 4.65(+1)  |           |           |        |
| 2-Fluorobenzoic acid                   | 3.27      |           |           |        |
| 3-Fluorobenzoic acid                   | 3.865     |           |           |        |
| 4-Fluorobenzoic acid                   | 4.14      |           |           |        |
| Fluoromandelic acid                    | 4.244     |           |           |        |
| 2-Fluorophenol                         | 8.73      |           |           |        |
| 3-Fluorophenol                         | 9.29      |           |           |        |
| 4-Fluorophenol                         | 9.89      |           |           |        |
| 2-Fluorophenoxyacetic acid             | 3.08      |           |           |        |
| 3-Fluorophenoxyacetic acid             | 3.08      |           |           |        |
| 4-Fluorophenoxyacetic acid             | 3.13      |           |           |        |
| 4-Fluorophenylacetic acid              | 4.25      |           |           |        |
| 2'-Fluorophenylalanine                 | 2.14(+1)  | 9.01(0)   |           |        |
| 3'-Fluorophenylalanine                 | 2.10(+1)  | 8.98(0)   |           |        |
| 4-Fluorophenylalanine                  | 2.13(+1)  | 9.05(0)   |           |        |
| 2-Fluorophenylphosphonic acid          | 1.64      | 6.80      |           |        |
| 3-Fluorophenylselenic acid             | 4.34      |           |           |        |
| 4-Fluorophenylselenic acid             | 4.50      |           |           |        |
| 2-Fluoropyridine                       | -0.44(+1) |           |           |        |
| 3-Fluoropyridine                       | 2.97(+1)  |           |           |        |
| 5-Fluorouracil                         | 8.00(0)   | ca 13(-1) |           |        |
| Folic acid (pteroylglutamic acid)      | 8.26      |           |           |        |
| Formic acid                            | 3.751     |           |           |        |
| N-Formylglycine                        | 3.43      |           |           |        |
| 2-Formyl-3-hydroxypyridine (20°C)      | 3.40(+1)  | 6.95(OH)  |           |        |
| 4-Formyl-3-hydroxypyridine             | 4.05(+1)  | 6.77(OH)  |           |        |
| 2-Formyl-3-methoxypyridine (20°C)      | 3.89(+1)  | 12.95     |           |        |
| Formyl-3-methoxypyridine (20°C)        | 4.45(+1)  | 11.7      |           |        |
| D-(-)-Fructose                         | 12.03     |           |           |        |
| Fumaric acid                           | 3.10      | 4.60      |           |        |
| 2-Furancarboxylic acid (2-furoic acid) | 3.164     |           |           |        |
| D-(+)-Galactose                        | 12.35     |           |           |        |
| Galactose-1-phosphoric acid            | 1.00      | 6.17      |           |        |
| Glucoscorbic acid                      | 4.26      | 11.58     |           |        |
| D-Gluconic acid                        | 3.86      |           |           |        |
| $\alpha$ -D-(+)-Glucose                | 12.28     |           |           |        |
| $\alpha$ -D-Glucose-1-phosphate        | 1.11(0)   | 6.504(-1) |           |        |
| trans-Glutaconic acid                  | 3.77      | 5.08      |           |        |
| D-(-)-Glutamic acid                    | 2.162(+1) | 4.272(0)  | 9.358(-1) |        |
| L-Glutamic acid                        | 2.19(+1)  | 4.25(0)   | 9.67(-1)  |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                        | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$  |
|----------------------------------------------------------------------------------|-----------|-----------|-----------|---------|
| Glutamic acid, 1-ethyl ester                                                     | 3.85(+1)  | 7.84(0)   |           |         |
| Glutamic acid, 5-ethyl ester                                                     | 2.15(+1)  | 9.19(0)   |           |         |
| L-Glutamine ( $\mu = 0.2$ )                                                      | 2.17(+1)  | 9.13(0)   |           |         |
| Glutaric acid                                                                    | 3.77      | 6.08      |           |         |
| Glutaric acid monoamide                                                          | 4.600(0)  |           |           |         |
| Glutarimide                                                                      | 11.43     |           |           |         |
| Glutathione                                                                      | 2.12(+1)  | 3.53(0)   | 8.66      | 9.12    |
| DL-Glyceric acid                                                                 | 3.64      |           |           |         |
| Glycerol                                                                         | 14.15     |           |           |         |
| Glyceryl-1-phosphoric acid                                                       | —         | 6.656(−1) |           |         |
| Glyceryl-2-phosphoric acid                                                       | 1.335(0)  | 6.650(−1) |           |         |
| Glycine                                                                          | 2.341(+1) | 9.60(0)   |           |         |
| Glycine amide                                                                    | 8.03(+1)  |           |           |         |
| Glycine, ethyl ester                                                             | 7.66(+1)  |           |           |         |
| Glycine hydroxamic acid                                                          | 7.10      | 9.10      |           |         |
| Glycine, methyl ester                                                            | 7.59(+1)  |           |           |         |
| Glycine-O-phenylphosphorylserine                                                 | 2.96      | 8.07      |           |         |
| Glycolic acid                                                                    | 3.831     |           |           |         |
| N-Glycl- $\alpha$ -alanine                                                       | 3.15(+1)  | 8.33(0)   |           |         |
| Glycylalanylalanine                                                              | 3.38(+1)  | 8.10(0)   |           |         |
| N-Glycylasparagine                                                               | 2.942     |           |           |         |
| Glycyclaspartic acid                                                             | 2.81(+1)  | 4.45(0)   | 8.60(−1)  |         |
| Glycyl-DL-glutamine (18°C)                                                       | 2.88(+1)  | 8.33(0)   |           |         |
| N-Glycylglycine                                                                  | 3.126(+1) | 8.252(0)  |           |         |
| Glycylglycylcysteine (35°C)                                                      | 2.71      | 2.71      | 7.94      | 7.94    |
| Glycylglycylglycine                                                              | 3.225(+1) | 8.090(0)  |           |         |
| Glycyl-L-histidine ( $\mu = 0.16$ )                                              | 6.79      | 8.20      |           |         |
| Glycylisoleucine                                                                 | 8.00      |           |           |         |
| N-Glycyl-L-leucine                                                               | 3.180(+1) | 8.327(0)  |           |         |
| Glycyl-O-phosphorylserine                                                        | 2.90      | 6.02      | 8.43      |         |
| L-Glycylproline ( $\mu = 0.1$ )                                                  | 2.81(+1)  | 8.65(0)   |           |         |
| N-Glycylsarcosine ( $\mu = 0.1$ )                                                | 2.98(+1)  | 8.55(0)   |           |         |
| N-Glycylserine                                                                   | 2.98(+1)  | 8.38(0)   |           |         |
| Glycylserylglycine                                                               | 3.32      | 7.99      |           |         |
| Glycyltyrosine                                                                   | 2.93      | 8.45      | 10.49     |         |
| Glycylvaline                                                                     | 3.15      | 8.18      |           |         |
| Glyoxaline                                                                       | 7.03(+1)  |           |           |         |
| Glyoxylic acid                                                                   | 3.30(0)   |           |           |         |
| Guanidineacetic acid                                                             | 2.82(+1)  |           |           |         |
| Guanine                                                                          | 3.3(+1)   | 9.2       | 12.3      |         |
| Guanine deoxyriboside-3'-phosphoric acid                                         | —         | 2.9       | 6.4       | 9.7     |
| Guanosine                                                                        | 1.9(+1)   | 9.25(0)   | 12.33(OH) |         |
| Guanosine-5'-diphosphoric acid ( $\mu = 0.1$ ; $pK_5$ 9.6)                       | —         | —         | 2.9       | 6.3     |
| Guanosine-3'-phosphoric acid                                                     | 0.7       | 2.3       | 5.92      | 9.38    |
| Guanosine-5'-phosphoric acid ( $\mu = 0.1$ )                                     | —         | 2.4       | 6.1       | 9.4     |
| Guanosine-5'-triphosphoric acid [ $\mu = 0.1$ ; $pK_5$ 7.10(−3); $pK_6$ 9.3(−4)] | —         | —         | —         | 3.0(−2) |
| Guanylurea                                                                       | 1.80      | 8.20      |           |         |
| Harmine (20°C)                                                                   | 7.61(+1)  |           |           |         |
| Heptafluorobutanoic acid                                                         | 0.17      |           |           |         |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                         | $pK_1$                      | $pK_2$     | $pK_3$   | $pK_4$    |
|---------------------------------------------------|-----------------------------|------------|----------|-----------|
| 4,4,5,5,6,6,6-Heptafluorohexanoic acid            | 4.18                        |            |          |           |
| 4,4,5,5,6,6,6-Heptafluoro-2-hexenoic acid         | 3.23                        |            |          |           |
| Heptanedioic acid (pimelic acid)                  | 4.484                       | 5.424      |          |           |
| 2,4-Heptanedione                                  | 8.43(keto);<br>9.15(enol)   |            |          |           |
| Heptanoic acid                                    | 4.893                       |            |          |           |
| Heroin                                            | 7.6(+1)                     |            |          |           |
| 2,4-Hexadienoic acid (sorbic acid)                | 4.77                        |            |          |           |
| 1,1,1,3,3,3-Hexafluoro-2,2-propanediol            | 8.801                       |            |          |           |
| 1,1,1,3,3,3-Hexafluoro-2-propanol                 | 9.42                        |            |          |           |
| Hexahydroazepine                                  | 11.07                       |            |          |           |
| Hexamethyldisilazine                              | 7.55                        |            |          |           |
| 1,2,3,8,9,10-Hexamethyl-4,7-phenanthroline (20°C) | 7.26                        |            |          |           |
| 1,6-Hexanediamine                                 | 9.830(+2)                   | 10.930(+1) |          |           |
| 1,6-Hexanedioic acid                              | 4.418                       | 5.412      |          |           |
| 2,4-Hexanedione                                   | 8.49 (enol);<br>9.32 (keto) |            |          |           |
| 2,2',4,4',6,6'-Hexanitrodiphenylamine             | 5.42(+1)                    |            |          |           |
| Hexanoic acid (20°C)                              | 4.849                       |            |          |           |
| <i>trans</i> -2-Hexenoic acid                     | 4.74                        |            |          |           |
| <i>trans</i> -3-Hexenoic acid                     | 4.72                        |            |          |           |
| 3-Hexen-4-oic acid                                | 4.58                        |            |          |           |
| 4-Hexen-5-oic acid                                | 4.74                        |            |          |           |
| Hexylamine                                        | 10.64(+1)                   |            |          |           |
| Hexylarsonic acid                                 | 4.16                        | 9.19       |          |           |
| Hexylphosphonic acid                              | 2.6                         | 7.9        |          |           |
| <b>DL</b> -Histidine                              | 1.82(+2)                    | 6.00(+1)   | 9.16(0)  |           |
| Histidine amide ( $\mu = 0.2$ )                   | 5.78(+2)                    | 7.64(+1)   |          |           |
| Histidine, methyl ester ( $\mu = 0.1$ )           | 5.01(+2)                    | 7.23(+1)   |          |           |
| Histidylglycine                                   | 2.40(+2)                    | 5.80(+1)   | 7.82(0)  |           |
| Histidylhistidine ( $\mu = 0.16$ )                | 5.40(+2)                    | 6.80(+1)   | 7.95(0)  |           |
| <b>DI</b> -Homatropine                            | 9.7(+1)                     |            |          |           |
| <b>DI</b> -Homocysteine                           | 2.222(+1)                   | 8.87       | 10.86    |           |
| Homocysteine ( $\mu = 0.1$ )                      | 1.593(+2)                   | 2.523(+1)  | 8.676(0) | 9.413(-1) |
| Hydantoin                                         | 9.12                        |            |          |           |
| Hydrastine                                        | 6.23(+1)                    |            |          |           |
| Hydrazine- <i>N,N</i> -diacetic acid              | <0.1                        | 2.8        | 3.8      |           |
| Hydrazine- <i>N'</i> - <i>N'</i> -diacetic acid   | 2.40                        | 3.12       | 7.32     |           |
| 4-Hydrazinocarbonylpyridine (20°C)                | 1.82                        | 3.52       | 10.79    |           |
| <i>N</i> -Hydroxyacetamide                        | 9.40                        |            |          |           |
| 2'-Hydroxyacetophenone                            | 9.90                        |            |          |           |
| 3'-Hydroxyacetophenone                            | 9.19                        |            |          |           |
| 4'-Hydroxyacetophenone                            | 8.05                        |            |          |           |
| 1-Hydroxyacridine (15°C)                          | 5.72                        |            |          |           |
| 2-Hydroxyacridine (15°C)                          | 5.62                        |            |          |           |
| 3-Hydroxyacridine (15°C)                          | 5.30                        |            |          |           |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                      | $pK_1$   | $pK_2$    | $pK_3$   | $pK_4$ |
|--------------------------------------------------------------------------------|----------|-----------|----------|--------|
| $\alpha$ -Hydroxyasparagine                                                    | 2.28(+1) | 7.20(0)   | 9.11(−1) |        |
| $\beta$ -Hydroxyasparagine                                                     | 2.09(+1) | 8.29(0)   |          |        |
| Hydroxyaspartic acid                                                           | 1.91(+1) | 3.51(0)   |          |        |
| 2-Hydroxybenzaldehyde (salicyl-<br>aldehyde)                                   | 8.34     |           | 12.11    |        |
| 3-Hydroxybenzaldehyde                                                          | 9.00     |           |          |        |
| 4-Hydroxybenzaldehyde                                                          | 7.620    |           |          |        |
| 2-Hydroxybenzaldehyde oxime                                                    | 1.37(+1) | 9.18      |          |        |
| 2-Hydroxybenzamide                                                             | 8.36     |           |          |        |
| 2-Hydroxybenzenemethanol (2-hy-<br>droxybenzyl alcohol)                        | 9.92     |           |          |        |
| 3-Hydroxybenzenemethanol                                                       | 9.83     |           |          |        |
| 4-Hydroxybenzenemethanol                                                       | 9.82     |           |          |        |
| 4-Hydroxybenzenesulfonic acid                                                  | —        | 9.055(−1) |          |        |
| 2-Hydroxybenzohydroxamic acid                                                  | 5.19     |           |          |        |
| 2-Hydroxybenzoic acid (salicylic<br>acid)                                      | 2.98     | 12.38     |          |        |
| 3-Hydroxybenzoic acid                                                          | 4.076    | 9.85      |          |        |
| 4-Hydroxybenzoic acid                                                          | 4.582    | 9.23      |          |        |
| 4-Hydroxybenzonitrile                                                          | 7.95     |           |          |        |
| 2-Hydroxy-5-bromobenzoic acid                                                  | 2.61     |           |          |        |
| 2-Hydroxybutanoic acid (30°C)                                                  | 3.65     |           |          |        |
| L-3-Hydroxybutanoic acid (30°C)                                                | 4.41     |           |          |        |
| 4-Hydroxybutanoic acid (30°C)                                                  | 4.71     |           |          |        |
| 2-Hydroxy-5-chlorobenzoic acid                                                 | 2.63     |           |          |        |
| <i>trans</i> -2'-Hydroxycinnamic acid                                          | 4.614    |           |          |        |
| <i>trans</i> -3'-Hydroxycinnamic acid                                          | 4.40     |           |          |        |
| 10-Hydroxycodeine                                                              | 7.12     |           |          |        |
| <i>cis</i> -2-Hydroxycyclohexane-1-car-<br>boxylic acid                        | 4.796    |           |          |        |
| <i>trans</i> -2-Hydroxycyclohexane-1-<br>carboxylic acid                       | 4.682    |           |          |        |
| <i>cis</i> -3-Hydroxycyclohexane-1-car-<br>boxylic acid                        | 4.602    |           |          |        |
| <i>trans</i> -3-Hydroxycyclohexane-1-<br>carboxylic acid                       | 4.815    |           |          |        |
| <i>cis</i> -4-Hydroxycyclohexane-1-car-<br>boxylic acid                        | 4.836    |           |          |        |
| <i>trans</i> -4-Hydroxycyclohexane-1-<br>carboxylic acid                       | 4.687    |           |          |        |
| 1-Hydroxy-2,4-dihydroxymethyl-<br>benzene                                      | 9.79     |           |          |        |
| <i>N</i> -(Hydroxyethyl)biguanide                                              | 2.8(+2)  | 11.53(+1) | 9.93     |        |
| <i>N</i> -(2-Hydroxy-<br>ethyl)ethylenediamine                                 | 7.21(+2) | 10.12(+1) |          |        |
| <i>N'</i> -(2-Hydroxyethyl)ethylenediam-<br>ine- <i>N,N,N'</i> -triacetic acid | 2.39     | 5.37      |          |        |
| <i>N</i> -(2-Hydroxyethyl)iminodiacetic<br>acid ( $\mu = 0.1$ )                | 2.2      | 8.65      |          |        |
| <i>N</i> -(2-Hydroxyethyl)piperazine- <i>N'</i> -<br>ethansulfonic acid (20°C) | 7.55     |           |          |        |
| 4'-(2-Hydroxyethyl)-1'-piperazine-<br>propanesulfonic acid (20°C)              | 8.00     |           |          |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                              | $pK_1$    | $pK_2$    | $pK_3$  | $pK_4$ |
|--------------------------------------------------------|-----------|-----------|---------|--------|
| 2-Hydroxyethyltrimethylamine                           | 8.94(+1)  |           |         |        |
| L- $\beta$ -Hydroxyglutamic acid                       | 2.09      | 4.18      | 9.20    |        |
| 1-Hydroxy-4-hydroxymethylbenzene                       | 9.84      |           |         |        |
| 5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one             | 7.90      | 8.03      |         |        |
| 3-Hydroxy-2-hydroxymethylpyridine (20°C, $\mu = 0.2$ ) | 5.00(+1)  | 9.07(OH)  |         |        |
| 3-Hydroxy-4-hydroxymethylpyridine (20°C, $\mu = 0.2$ ) | 5.00(+1)  | 8.95(OH)  |         |        |
| 8-Hydroxy-7-iodoquinoline-5-sulfonic acid              | 2.51(0)   | 7.417(−1) |         |        |
| Hydroxylysine (38°C, $\mu = 0.1$ )                     | 2.13(+2)  | 8.62(+1)  | 9.67(0) |        |
| 2-Hydroxy-3-methoxybenzaldehyde                        | 7.912     |           |         |        |
| 3-Hydroxy-4-methoxybenzaldehyde (isovanillin)          | 8.889     |           |         |        |
| 4-Hydroxy-3-methoxybenzaldehyde (vanillin)             | 7.396     |           |         |        |
| 4-Hydroxy-3-methoxybenzoic acid                        | 4.355     |           |         |        |
| 1-Hydroxy-2-methoxybenzylamine                         | 8.70(+1)  | 10.52(0)  |         |        |
| 2-Hydroxy-1-methoxybenzylamine                         | 8.89(+1)  | 10.52(0)  |         |        |
| 3-Hydroxy-2-methoxybenzylamine                         | 8.94(+1)  | 10.42(0)  |         |        |
| 2-Hydroxymethyl-2-benzeneacetic acid                   | 4.12      |           |         |        |
| (2-Hydroxy-5-methylbenzene)-methanol                   | 10.15     |           |         |        |
| 2-Hydroxy-3-methylbenzoic acid                         | 2.99      |           |         |        |
| 2-Hydroxy-4-methylbenzoic acid                         | 3.17      |           |         |        |
| 2-Hydroxy-5-methylbenzoic acid                         | 4.08      |           |         |        |
| 2-Hydroxy-6-methylbenzoic acid                         | 3.32      |           |         |        |
| 2-Hydroxy-2-methylbutanoic acid (18°C)                 | 3.991     |           |         |        |
| 3-Hydroxy-2-methylbutanoic acid (18°C)                 | 4.648     |           |         |        |
| 4-Hydroxy-4-methylpentanoic acid (18°C)                | 4.873     |           |         |        |
| 1-Hydroxymethylphenol                                  | 9.95      |           |         |        |
| Hydroxymethylphosphoric acid                           | 1.91      | 7.15      |         |        |
| 2-Hydroxy-2-methylpropanoic acid ( $\mu = 0.1$ )       | 3.717     |           |         |        |
| 2-Hydroxy-4-methylpyridine                             | 4.529(+1) |           |         |        |
| 8-Hydroxy-2-methylquinoline                            | 5.55(+1)  | 10.31(0)  |         |        |
| 8-Hydroxy-4-methylquinoline                            | 5.56(+1)  | 10.00(0)  |         |        |
| 8-Hydroxy-2-methylquinoline-5-sulfonic acid            | 4.80(0)   | 9.30(−1)  |         |        |
| 8-Hydroxy-4-methylquinoline-7-sulfonic acid            | 4.78(0)   | 10.01(−1) |         |        |
| 8-Hydroxy-6-methylquinoline-5-sulfonic acid            | 4.20(0)   | 8.7(−1)   |         |        |
| 2-Hydroxy-1-naphthoic acid (20°C)                      | 3.29      | 9.68      |         |        |
| 2-Hydroxy-2-nitrobenzoic acid                          | 2.23      |           |         |        |
| 2-Hydroxy-3-nitrobenzoic acid                          | 1.87      |           |         |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                             | $pK_1$    | $pK_2$           | $pK_3$   | $pK_4$ |
|-------------------------------------------------------|-----------|------------------|----------|--------|
| 2-Hydroxy-5-nitrobenzoic acid                         | 2.12      |                  |          |        |
| 2-Hydroxy-6-nitrobenzoic acid                         | 2.24      |                  |          |        |
| 2-Hydroxy-4-nitrophenylphosphonic acid                | 1.22      | 5.39             |          |        |
| 8-Hydroxy-7-nitroquinoline-5-sulfonic acid            | 1.94(0)   | 5.750(−1)        |          |        |
| 3-Hydroxy-4-nitrotoluene ( $\mu = 0.1$ )              | 7.41      |                  |          |        |
| 4-Hydroxypentanoic acid (18°C)                        | 4.686     |                  |          |        |
| 4-Hydroxy-3-pentenoic acid                            | 4.30      |                  |          |        |
| 3-Hydroxyphenazine (15°C)                             | 2.67      |                  |          |        |
| 4-Hydroxyphenylarsonic acid                           | 3.89      | 8.37<br>(phenol) | 10.05    |        |
| 3-Hydroxyphenylboric acid                             | 8.55      | 10.84            |          |        |
| 2-Hydroxy-2-phenylpropanoic acid                      | 3.532     |                  |          |        |
| 2-(2-Hydroxyphenyl)pyridine (20°C)                    | 4.19(+1)  | 10.64            |          |        |
| <i>trans</i> -4-Hydroxyproline                        | 1.818(+1) | 9.662(0)         |          |        |
| Hydroxypropanedioic acid (tartronic acid)             | 2.37      | 4.74             |          |        |
| 2-Hydroxypropanoic acid                               | 3.858     |                  |          |        |
| 1-Hydroxy-2-propylbenzene                             | 10.50     |                  |          |        |
| 4-Hydroxypteridine                                    | 1.3(+1)   | 7.89(0)          |          |        |
| 2-Hydroxypyridine                                     | 1.25(+1)  | 11.62(0)         |          |        |
| 3-Hydroxypyridine                                     | 4.80(+1)  | 8.72(0)          |          |        |
| 4-Hydroxypyridine                                     | 3.23(+1)  | 11.09(0)         |          |        |
| 2-Hydroxypyridine- <i>N</i> -oxide                    | −0.62(+1) | 5.97(0)          |          |        |
| 2-Hydroxypyrimidine                                   | 2.24(+1)  | 9.17(0)          |          |        |
| 4-Hydroxypyrimidine                                   | 1.85(+1)  | 8.59(0)          |          |        |
| 8-Hydroxyquinazoline                                  | 3.41(+1)  | 8.65(0)          |          |        |
| 2-Hydroxyquinoline (20°C)                             | −0.31(+1) | 11.74            |          |        |
| 3-Hydroxyquinoline (20°C)                             | 4.30(+1)  | 8.06(0)          |          |        |
| 4-Hydroxyquinoline (20°C)                             | 2.27(+1)  | 11.25(0)         |          |        |
| 5-Hydroxyquinoline (20°C)                             | 5.20(+1)  | 8.54(0)          |          |        |
| 6-Hydroxyquinoline (20°C)                             | 5.17(+1)  | 8.88(0)          |          |        |
| 7-Hydroxyquinoline (20°C)                             | 5.48(+1)  | 8.85(0)          |          |        |
| 8-Hydroxyquinoline (20°C)                             | 4.91(+1)  | 9.81(0)          |          |        |
| 8-Hydroxyquinoline-5-sulfonic acid                    | 4.092(+1) | 8.776(0)         |          |        |
| <b>DL</b> -Hydroxysuccinic acid (malic acid)          | 3.458     | 5.097            |          |        |
| <b>L</b> -Hydroxysuccinic acid                        | 3.40      | 5.05             |          |        |
| Hydroxytetracycline                                   | 3.27(+1)  | 7.32(0)          | 9.11(−1) |        |
| 5-Hydroxy-1,2,3,4-tetrazole                           | 3.32      |                  |          |        |
| 4-Hydroxy-3-(2'-thiazolyazo)toluene                   | 8.36      |                  |          |        |
| 2-Hydroxytoluene                                      | 10.33     |                  |          |        |
| 3-Hydroxytoluene                                      | 10.10     |                  |          |        |
| 4-Hydroxytoluene                                      | 10.276    |                  |          |        |
| 4-Hydroxy- $\alpha, \alpha, \alpha$ -trifluorotoluene | 8.675     |                  |          |        |
| 1-Hydroxy-2,4,6-trihydroxymethylbenzene               | 9.56      |                  |          |        |
| Hydroxyuracil                                         | 8.64      |                  |          |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                | pK <sub>1</sub> | pK <sub>2</sub>                 | pK <sub>3</sub>     | pK <sub>4</sub> |  |
|----------------------------------------------------------|-----------------|---------------------------------|---------------------|-----------------|--|
| Hydroxyvaline                                            | 2.55(+1)        | 9.77(0)                         | 12.07(−1)           |                 |  |
| Hyoscyamine                                              | 9.68(+1)        |                                 |                     |                 |  |
| Hypoxanthene                                             | 1.79(+1)        | 8.91(0)                         |                     |                 |  |
| Hypoxanthine                                             | 5.3             |                                 |                     |                 |  |
| Imidazole                                                | 6.993(+1)       | 10.58(0)                        | 10.70(0)            |                 |  |
| Imidazolidinetrione (parabanic acid)                     | 6.10            |                                 |                     |                 |  |
| 4-(4-Imidazolyl)butanoic acid (μ = 0.1)                  | 4.26(+1)        | 7.26(0)                         |                     |                 |  |
| 2-(4-Imidazolyl)ethylamine                               | 5.784(+2)       | 9.756(+1)                       |                     |                 |  |
| 3-(4-Imidazolyl)propanoic acid (μ = 0.16)                | 3.96(+1)        | 7.57(0)                         |                     |                 |  |
| 3,3′-Iminobispropanoic acid                              | 4.11(0)         | 9.61(−1)                        |                     |                 |  |
| 3,3′-Iminobispropylamine (30°C)                          | 8.02(+2)        | 9.70(+1)                        |                     |                 |  |
| 2,2′-Iminodiacetic acid (diglycine) (30°C, μ = 0.1)      | 2.54(0)         | 9.12(−1)                        |                     |                 |  |
| 4-Indanol                                                | 10.32           |                                 |                     |                 |  |
| Indole-3-acetic acid                                     | 4.75            |                                 |                     |                 |  |
| Inosine                                                  | ca 1.5(+1)      | 8.96(0)                         | 12.36               | 6.92(−3)        |  |
| Inosine-5′-phosphoric acid                               | 1.54(0)         | 6.66(−1)                        | 2.2(−2)             |                 |  |
| Inosine-5′-triphosphoric acid [pK <sub>5</sub> 7.68(−4)] | —               | —                               |                     |                 |  |
| Iodoacetic acid                                          | 3.175           |                                 | 11.88(0)<br>(imino) |                 |  |
| 2-Iodoaniline                                            | 2.54(+1)        |                                 |                     |                 |  |
| 3-Iodoaniline                                            | 3.58(+1)        |                                 |                     |                 |  |
| 4-Iodoaniline                                            | 3.82(+1)        |                                 |                     |                 |  |
| 2-Iodobenzoic acid                                       | 2.86            |                                 |                     |                 |  |
| 3-Iodobenzoic acid                                       | 3.86            |                                 |                     |                 |  |
| 4-Iodobenzoic acid                                       | 4.00            |                                 |                     |                 |  |
| 5-Iodohistamine                                          | 4.06(+1)        | 9.20(+1)                        |                     |                 |  |
|                                                          | (imidazole)     | (NH <sub>3</sub> <sup>+</sup> ) |                     |                 |  |
| 7-Iodo-8-hydroxyquinoline-5-sulfonic acid                | 2.514           | 7.417                           |                     |                 |  |
| Iodomandelic acid                                        | 3.264           |                                 | 7.06                |                 |  |
| Iodomethylphosphoric acid                                | 1.30            | 6.72                            |                     |                 |  |
| 2-Iodophenol                                             | 8.464           |                                 |                     |                 |  |
| 3-Iodophenol                                             | 8.879           |                                 |                     |                 |  |
| 4-Iodophenol                                             | 9.200           |                                 |                     |                 |  |
| 2-Iodophenoxyacetic acid                                 | 3.17            |                                 |                     |                 |  |
| 3-Iodophenoxyacetic acid                                 | 3.13            |                                 |                     |                 |  |
| 4-Iodophenoxyacetic acid                                 | 3.16            |                                 |                     |                 |  |
| 2-Iodophenylacetic acid                                  | 4.038           |                                 |                     |                 |  |
| 3-Iodophenylacetic acid                                  | 4.159           |                                 |                     |                 |  |
| 4-Iodophenylacetic acid                                  | 4.178           |                                 |                     |                 |  |
| 2-Iodophenylphosphoric acid                              | 1.74            | 7.06                            |                     |                 |  |
| 2-Iodopropanoic acid                                     | 3.11            |                                 | 8.02(0)             |                 |  |
| 3-Iodopropanoic acid                                     | 4.08            |                                 |                     |                 |  |
| 2-Iodopyridine                                           | 1.82(+1)        |                                 |                     |                 |  |
| 3-Iodopyridine                                           | 3.25(+1)        |                                 |                     |                 |  |
| 4-Iodopyridine (20°C)                                    | 4.02(+1)        |                                 |                     |                 |  |
| Isoasparagine                                            | 2.97(+1)        | 8.02(0)                         |                     |                 |  |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                  | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$    |
|--------------------------------------------|-----------|-----------|-----------|-----------|
| Isobutylacetic acid (18°C)                 | 4.79      |           |           |           |
| Isobutylamine                              | 10.41(+1) |           |           |           |
| Isochlorotetracycline                      | 3.1(+1)   | 6.7(0)    | 8.3(−1)   |           |
| Isocreatine                                | 2.84(+1)  |           |           |           |
| Isogluatamine                              | 3.81(+1)  | 7.88(0)   |           |           |
| Isohistamine ( $\mu = 0.1$ )               | 6.036(+2) | 9.274(+1) |           |           |
| L-Isoleucine                               | 2.35(+1)  | 9.68(0)   |           |           |
| Isolysergic acid                           | 3.33(0)   | 8.46(NH)  |           |           |
| Isopilocarpine (15°C)                      | 7.18(+1)  |           |           |           |
| 2-(Isopropoxy)benzoic acid (20°C)          | 4.24      |           |           |           |
| 3-(Isopropoxy)benzoic acid (20°C)          | 4.15      |           |           |           |
| 4-(Isopropoxy)benzoic acid (20°C)          | 4.68      |           |           |           |
| Isopropylamine                             | 10.64(+1) |           |           |           |
| N-Isopropylaniline                         | 5.50(+1)  |           |           |           |
| 5-Isopropylbarbituric acid                 | 4.907(+1) |           |           |           |
| 2-Isopropylbenzene acid                    | 3.64      |           |           |           |
| 4-Isopropylbenzene acid                    | 4.36      |           |           |           |
| N-Isopropylglycine ( $\mu = 0.1$ )         | 2.36(+1)  | 10.06(0)  |           |           |
| Isopropylmalonic acid                      | 2.94      | 5.88      |           |           |
| Isopropylmalonic acid mononitrile          | 2.401     |           |           |           |
| 3-Isopropyl-4-(methylamino)pyridine (20°C) | 9.96(+1)  |           |           |           |
| 3-Isopropylpentanedioic acid               | 4.30      | 5.51      |           |           |
| 4-Isopropylphenylacetic acid               | 4.391     |           |           |           |
| Isopropylphosphinic acid                   | 3.56      |           |           |           |
| Isopropylphosphonic acid                   | 2.66      | 8.44      |           |           |
| 2-Isopropylpyridine                        | 5.83(+1)  |           |           |           |
| 3-Isopropylpyridine (20°C)                 | 5.72(+1)  |           |           |           |
| 4-Isopropylpyridine                        | 6.02(+1)  |           |           |           |
| DL-Isoproterenol                           | 8.64(+1)  |           |           |           |
| Isoquinoline                               | 5.40(+1)  |           |           |           |
| Isoretronecanol                            | 10.83     |           |           |           |
| L-Isoserine ( $\mu = 0.16$ )               | 2.72(+1)  | 9.25(0)   |           |           |
| Isothiocyanatoacetic acid                  | 6.62      |           |           |           |
| L-(+)-Lactic acid                          | 3.858     |           |           |           |
| L-Leucine                                  | 2.33(+1)  | 9.60(0)   |           |           |
| Leucine amide                              | 7.80(+1)  |           |           |           |
| Leucine, ethyl ester ( $\mu = 0.1$ )       | 7.57(+1)  |           |           |           |
| L-Leucyl-L-asparagine                      | 3.00(+1)  | 8.12(0)   |           |           |
| L-Leucyl-L-glutamine                       | 2.99(+1)  | 8.11(0)   |           |           |
| DL-Leucylglycine                           | 3.25(+1)  | 8.28(0)   |           |           |
| Leucylisoserine (20°C)                     | 3.188(+1) | 8.207(0)  |           |           |
| D-Leucyl-L-tyrosine                        | 3.12(+1)  | 8.38(0)   | 10.35(−1) |           |
| L-Leucyl-L-tyrosine                        | 3.46(+1)  | 7.84(0)   | 10.09(−1) |           |
| Lysergic acid                              | 3.44(+1)  | 7.68(0)   |           |           |
| L-(+)-Lysine                               | 2.18(+2)  | 8.94(+1)  | 10.53(0)  |           |
| Lysine, methyl ester ( $\mu = 0.1$ )       | 6.965(+1) | 10.251(0) |           |           |
| L-Lysyl-L-alanine                          | 3.22(+1)  | 7.62(0)   | 10.70(−1) |           |
| L-Lysyl-D-alanine                          | 3.00(+1)  | 7.74(0)   | 10.63(−1) |           |
| Lysylglutamic acid                         | 2.93(+2)  | 4.47(+1)  | 7.75(0)   | 10.50(+1) |
| L-Lysyl-L-lysine ( $\mu = 0.1$ )           | 3.01(+2)  | 7.53(+1)  | 10.05(0)  | 10.01(−1) |



**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                    | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$    |
|----------------------------------------------|-----------|-----------|-----------|-----------|
| L-Lysyl-D-lysine ( $\mu = 0.1$ )             | 2.85(+2)  | 7.53(+1)  | 9.92(0)   | 10.89(−1) |
| L-Lysyl-L-lysyl-L-lysine ( $\mu = 0.1$ )     | 3.08(+2)  | 7.34(+1)  | 9.80(0)   | 10.54(−1) |
| L-Lysyl-D-lysyl-L-lysine ( $\mu = 0.1$ )     | 2.91(+2)  | 7.29(+1)  | 9.79(0)   | 10.54(−1) |
| L-Lysyl-D-lysyl-lysine ( $\mu = 0.1$ )       | 2.94(+2)  | 7.15(+1)  | 9.60(0)   | 10.38(−1) |
| $\alpha$ -D-Lyxose                           | 12.11     |           |           |           |
| Maleic acid                                  | 1.910     | 6.33      |           |           |
| Malonamic acid                               | 3.641(0)  |           |           |           |
| Malonic acid                                 | 2.826     | 5.696     |           |           |
| Malonitrile (cyanoacetic acid)               | 2.460     |           |           |           |
| Mandelic acid                                | 3.411     |           |           |           |
| D-(+)-Mannose                                | 12.08     |           |           |           |
| Mercaptoacetic acid (thioglycolic acid)      | 3.60(0)   | 10.56(SH) |           |           |
| 2-Mercaptobenzoic acid (20°C)                | 4.05(0)   |           |           |           |
| 2-Mercaptobutanoic acid                      | 3.53(0)   |           |           |           |
| Mercaptodiacetic acid                        | 3.32      | 4.29      |           |           |
| 2-Mercaptoethanesulfonic acid (20°C)         |           | 9.5(−1)   |           |           |
| 2-Mercaptoethanol                            | 9.88      |           |           |           |
| 2-Mercaptoethylamine                         | 8.27(+1)  | 10.53(0)  |           |           |
| 2-Mercaptohistidine                          | 1.84(+1)  | 8.47(0)   | 11.4(SH)  |           |
| Mercapto-S-phenylacetic acid ( $\mu = 0.1$ ) | 3.9       |           |           |           |
| 2-Mercaptopropane ( $\mu = 0.1$ )            | 10.86     |           |           |           |
| 3-Mercapto-1,2-propanediol ( $\mu = 0.5$ )   | 9.43      |           |           |           |
| 2-Mercaptopropanoic acid                     | 4.32(0)   | 10.20(SH) |           |           |
| 3-Mercaptopropanoic acid                     | —         | 10.84(SH) |           |           |
| 2-Mercaptopyridine (20°C)                    | −1.07(+1) | 10.00(0)  |           |           |
| 3-Mercaptopyridine (20°C)                    | 2.26(+1)  | 7.03(0)   |           |           |
| 4-Mercaptopyridine (20°C)                    | 1.43(+1)  | 8.86(0)   |           |           |
| 2-Mercaptoquinoline (20°C)                   | −1.44(+1) | 10.21(0)  |           |           |
| 3-Mercaptoquinoline (20°C)                   | 2.33(+1)  | 6.13(0)   |           |           |
| 4-Mercaptoquinoline (20°C)                   | 0.77(+1)  | 8.83(0)   |           |           |
| Mercaptosuccinic acid                        | 3.30(0)   | 4.94(−1)  | 10.94(SH) |           |
| Mesitylenic acid                             | 4.32      |           |           |           |
| Mesoxaldialdehyde                            | 3.60      |           |           |           |
| Methacrylic acid                             | 4.66      |           |           |           |
| Methanethiol                                 | 10.70     |           |           |           |
| DL-Methionine                                | 2.28(+1)  | 9.21(0)   |           |           |
| 2-(N-Methoxyacetamido)pyridine               | 2.01(+1)  |           |           |           |
| 3-(N-Methoxyacetamido)pyridine               | 3.52(+1)  |           |           |           |
| 4-(N-Methoxyacetamido)pyridine               | 4.62(+1)  |           |           |           |
| Methoxyacetic acid                           | 3.570     |           |           |           |
| 3-Methoxy-D- $\alpha$ -alanine               | 2.037(+1) | 9.176(0)  |           |           |
| 2-Methoxyaniline                             | 4.53(+1)  |           |           |           |
| 3-Methoxyaniline                             | 4.20(+1)  |           |           |           |
| 4-Methoxyaniline                             | 5.36(+1)  |           |           |           |
| 2-Methoxybenzoic acid                        | 4.09      |           |           |           |
| 3-Methoxybenzoic acid                        | 4.08      |           |           |           |
| 4-Methoxybenzoic acid                        | 4.49      |           |           |           |
| N,N-Methoxybenzylamine                       | 9.68(+1)  |           |           |           |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                             | $pK_1$    | $pK_2$   | $pK_3$ | $pK_4$ |
|-------------------------------------------------------|-----------|----------|--------|--------|
| 2-Methoxycarbonylaniline                              | 2.23(+1)  |          |        |        |
| 3-Methoxycarbonylaniline                              | 3.64(+1)  |          |        |        |
| 4-Methoxycarbonylaniline                              | 2.38(+1)  |          |        |        |
| Methoxycarbonylmethylamine                            | 7.66(+1)  |          |        |        |
| 2-Methoxycarbonylpyridine                             | 2.21(+1)  |          |        |        |
| 3-Methoxycarbonylpyridine                             | 3.13(+1)  |          |        |        |
| 4-Methoxycarbonylpyridine                             | 3.26(+1)  |          |        |        |
| <i>trans</i> -2-Methoxycinnamic acid                  | 4.462     |          |        |        |
| <i>trans</i> -3-Methoxycinnamic acid                  | 4.376     |          |        |        |
| <i>trans</i> -4-Methoxycinnamic acid                  | 4.539     |          |        |        |
| 2-Methoxyethylamine                                   | 9.45(+1)  |          |        |        |
| 2-Methoxy-4-nitrophenylphosphonic acid                | 1.53      | 6.96     |        |        |
| 2-Methoxyphenol                                       | 9.99      |          |        |        |
| 3-Methoxyphenol                                       | 9.652     |          |        |        |
| 4-Methoxyphenol                                       | 10.20     |          |        |        |
| (2'-Methoxy)phenoxyacetic acid                        | 3.231     |          |        |        |
| (3'-Methoxy)phenoxyacetic acid                        | 3.141     |          |        |        |
| (4'-Methoxy)phenoxyacetic acid                        | 3.213     |          |        |        |
| 4'-Methoxyphenylacetic acid                           | 4.358     |          |        |        |
| (4-Methoxyphenyl)phosphinic acid (17°C)               | 2.35      |          |        |        |
| (2-Methoxyphenyl)phosphonic acid                      | 2.16      | 7.77     |        |        |
| (4-Methoxyphenyl)phosphonic acid (17°C)               | 2.4       | 7.15     |        |        |
| 3-(2'-Methoxyphenyl)propanoic acid                    | 4.804     |          |        |        |
| 3-(3'-Methoxyphenyl)propanoic acid                    | 4.654     |          |        |        |
| 3-(4'-Methoxyphenyl)propanoic acid                    | 4.689     |          |        |        |
| 3-Methoxyphenylselenic acid                           | 4.65      |          |        |        |
| 4-Methoxyphenylselenic acid                           | 5.05      |          |        |        |
| 2-Methoxy-4-(2-propenyl)phenol                        | 10.0      |          |        |        |
| 2-Methoxypyridine                                     | 3.06(+1)  |          |        |        |
| 3-Methoxypyridine                                     | 4.91(+1)  |          |        |        |
| 4-Methoxypyridine                                     | 6.47(+1)  |          |        |        |
| 4-Methoxy-2-(2'-thiazoylazo)phenol                    | 7.83      |          |        |        |
| 2-Methylacrylic acid (18°C)                           | 4.66      |          |        |        |
| <i>N</i> -Methylalanine                               | 2.22(+1)  | 10.19(0) |        |        |
| <i>O</i> -Methylallothreonine ( $\mu = 0.1$ )         | 1.92(+1)  | 8.90(0)  |        |        |
| Methylamine                                           | 10.62(+1) |          |        |        |
| 2-( <i>N</i> -Methylamino)benzoic acid                | 1.93(+1)  | 5.34(0)  |        |        |
| 3-( <i>N</i> -Methylamino)benzoic acid                | —         | 5.10(0)  |        |        |
| 4-( <i>N</i> -Methylamino)benzoic acid                | —         | 5.05     |        |        |
| Methylaminodiacetic acid (20°C)                       | 2.146     | 10.088   |        |        |
| 2-(Methylamino)ethanol                                | 9.88(+1)  |          |        |        |
| 2-(2-Methylaminoethyl)pyridine (30°C)                 | 3.58(+2)  | 9.65(+1) |        |        |
| 2-(Methylaminomethyl)6-methylpyridine ( $\mu = 0.5$ ) | 3.03(+2)  | 9.15(+1) |        |        |
| 2-(Methylaminomethyl)pyridine (30°C)                  | 2.92(+2)  | 8.82(+1) |        |        |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                                | $pK_1$    | $pK_2$    | $pK_3$   | $pK_4$ |
|----------------------------------------------------------|-----------|-----------|----------|--------|
| 4-Methylamino-3-methylpyridine (20°C)                    | 9.83(+1)  |           |          |        |
| (3-Methylamino)phenylphosphonic acid                     | 1.1(+1)   | 4.72(+1)  | 7.30(−1) |        |
| (4-Methylamino)phenylphosphonic acid                     | —         | —         | 7.85(−1) |        |
| 3-(Methylamino)pyridine (30°C)                           | 8.70(+1)  |           |          |        |
| 4-(Methylamino)pyridine (20°C)                           | 9.65(+1)  |           |          |        |
| 4-(Methylamino)-2,3,5,6-tetra-methylpyridine (20°C)      | 10.06(+1) |           |          |        |
| <i>N</i> -Methylaniline                                  | 4.85(+1)  |           |          |        |
| Methylarsonic acid (18°C)                                | 3.41      | 8.18      |          |        |
| 1-Methylbarbituric acid                                  | 4.35(+1)  |           |          |        |
| 5-Methylbarbituric acid                                  | 3.386(+1) |           |          |        |
| 2-( <i>N</i> -Methylbenzamido)pyridine                   | 1.44(+1)  |           |          |        |
| 3-( <i>N</i> -Methylbenzamido)pyridine                   | 3.66(+1)  |           |          |        |
| 4-( <i>N</i> -Methylbenzamido)pyridine                   | 4.68(+1)  |           |          |        |
| 2-Methylbenzimidazole ( $\mu = 0.16$ )                   | 6.29(+1)  |           |          |        |
| 2-Methylbenzoic acid ( <i>o</i> -toluic acid)            | 3.90      |           |          |        |
| 3-Methylbenzoic acid                                     | 4.269     |           |          |        |
| 4-Methylbenzoic acid                                     | 4.362     |           |          |        |
| <i>N</i> -Methyl-1-benzoyllecgonine                      | 8.65      |           |          |        |
| Methylbiguanidine                                        | 3.00(+2)  | 11.44(+1) |          |        |
| 2-Methyl-2-butanethiol                                   | 11.35     |           |          |        |
| 2-Methylbutanoic acid                                    | 4.761     |           |          |        |
| 3-Methylbutanoic acid (20°C)                             | 4.767     |           |          |        |
| ( <i>E</i> )-2-Methyl-2-butendioic acid (mesaconic acid) | 3.09      | 4.75      |          |        |
| 3-Methyl-2-butenic acid                                  | 5.12      |           |          |        |
| ( <i>E</i> )-2-Methyl-2-butenic acid (tiglic acid)       | 4.96      |           |          |        |
| ( <i>Z</i> )-2-Methyl-2-butenic acid (angelic acid)      | 4.30      |           |          |        |
| 4-Methylcarboxylphenol                                   | 8.47      |           |          |        |
| ( <i>E</i> )-2-Methylcinnamic acid                       | 4.500     |           |          |        |
| ( <i>E</i> )-3-Methylcinnamic acid                       | 4.442     |           |          |        |
| ( <i>E</i> )-4-Methylcinnamic acid                       | 4.564     |           |          |        |
| 1-Methylcyclohexane-1-carboxylic acid                    | 5.13      |           |          |        |
| <i>cis</i> -2-Methylcyclohexane-1-carboxylic acid        | 5.03      |           |          |        |
| <i>trans</i> -2-Methylcyclohexane-1-carboxylic acid      | 5.73      |           |          |        |
| <i>cis</i> -3-Methylcyclohexane-1-carboxylic acid        | 4.88      |           |          |        |
| <i>trans</i> -3-Methylcyclohexane-1-carboxylic acid      | 5.02      |           |          |        |
| <i>cis</i> -4-Methylcyclohexane-1-carboxylic acid        | 5.04      |           |          |        |
| <i>trans</i> -4-Methylcyclohexane-1-carboxylic acid      | 4.89      |           |          |        |
| 2-Methylcyclohexyl-1,1-diacetic acid                     | 3.53      | 6.89      |          |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                     | $pK_1$                    | $pK_2$    | $pK_3$    | $pK_4$ |
|-----------------------------------------------|---------------------------|-----------|-----------|--------|
| 3-Methylcyclohexyl-1,1-diacetic acid          | 3.49                      | 6.08      |           |        |
| 4-Methylcyclohexyl-1,1,1-diacetic acid        | 3.49                      | 6.10      |           |        |
| 3-Methylcyclopentyl-1,1-diacetic acid         | 3.79                      | 6.74      |           |        |
| S-Methyl-L-cysteine                           | 8.97                      |           |           |        |
| N-Methylcytidine                              | 3.88                      |           |           |        |
| 5-Methylcytidine                              | 4.21                      |           |           |        |
| N-Methyl-2'-deoxycytidine                     | 3.97                      |           |           |        |
| 5-Methyl-2'-deoxycytidine                     | 4.33                      |           |           |        |
| 2-Methyl-3,5-dinitrobenzoic acid              | 2.97                      |           |           |        |
| 5-Methyldipropylenetriamine (30°C)            | 6.32(+3)                  | 9.19(+2)  | 10.33(+1) |        |
| 2,2'-Methylenebis(4-chlorophenol)             | 7.6                       | 11.5      |           |        |
| 2,2'-Methylenebis(4,6-dichlorophenol)         | 5.6                       | 10.56     |           |        |
| Methylenebis(thioacetic acid) (18°C)          | 3.310                     | 4.345     |           |        |
| 3,3'-(Methylenedithio)dialanine               | 2.200(+1)                 | 8.16(0)   |           |        |
| Methylenesuccinic acid                        | 3.85                      | 5.45      |           |        |
| N-Methylethylamine                            | 4.23(+1)                  |           |           |        |
| N-Methylethylenediamine                       | 6.86(+1)                  | 10.15(+1) |           |        |
| $\alpha$ -Methylglucoside                     | 13.71                     |           |           |        |
| 3-Methylglutaric acid                         | 4.24                      | 5.41      |           |        |
| N-Methylglycine (sarcosine)                   | 2.12(+1)                  | 10.20(0)  |           |        |
| 5-Methyl-2,4-heptanedione                     | 8.52(enol);<br>9.10(keto) |           |           |        |
| 5-Methyl-2,4-hexanedione                      | 8.66(enol);<br>9.31(keto) |           |           |        |
| 5-Methyl-4-hexenoic acid                      | 4.80                      |           |           |        |
| 3-Methylhistamine                             | 5.80(+1)                  | 9.90(0)   |           |        |
| 1-Methylhistidine                             | 1.69                      | 6.48      | 8.85      |        |
| 2-Methylhistidine (18°C)                      | 1.7                       | 7.2       | 9.5       |        |
| 2-Methyl-8-hydroxyquinoline ( $\mu = 0.005$ ) | 4.58(+1)                  | 11.71(0)  |           |        |
| 4-Methyl-8-hydroxyquinoline                   | 4.67(+1)                  | 11.62(0)  |           |        |
| 1-Methylimidazole                             | 7.06(+1)                  |           |           |        |
| 4-Methylimidazole                             | 7.55(+1)                  |           |           |        |
| N-Methyliminodiacetic acid                    | 2.15                      | 10.09     |           |        |
| S-Methylisothiourea                           | 9.83(+1)                  |           |           |        |
| O-Methylisourea                               | 9.72(+1)                  |           |           |        |
| Methylmalonic acid                            | 3.07                      | 5.87      |           |        |
| 2-(N-Methylmethanesulfonamido)pyridine        | 1.73(+1)                  |           |           |        |
| 3-(N-Methylmethanesulfonamido)pyridine        | 3.94(+1)                  |           |           |        |
| 4-(N-Methylmethanesulfonamido)pyridine        | 5.14(+1)                  |           |           |        |
| 2-Methyl-6-methylaminopyridine (20°C)         | 3.17(+1)                  | 8.84(0)   |           |        |
| 3-Methyl-4-methylaminopyridine (20°C)         | —                         | 9.84(0)   |           |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                          | $pK_1$     | $pK_2$    | $pK_3$ | $pK_4$ |
|----------------------------------------------------|------------|-----------|--------|--------|
| 4-Methyl-2,2'-(4-methylpyridyl)pyridine            | 5.32(+1)   |           |        |        |
| N-Methylmorpholine                                 | 7.13(+1)   |           |        |        |
| 2-Methyl-1-naphthoic acid                          | 3.11       |           |        |        |
| N-Methyl-1-naphthylamine                           | 3.70(+1)   |           |        |        |
| 2-Methyl-4-nitrobenzoic acid                       | 1.86       |           |        |        |
| 2-Methyl-6-nitrobenzoic acid                       | 1.87       |           |        |        |
| 1-Methyl-2-nitroterephthalic acid                  | 3.11       |           |        |        |
| 4-Methyl-2-nitroterephthalic acid                  | 1.82       |           |        |        |
| 3-Methylpentanedioic acid                          | 4.25       | 5.41      |        |        |
| 3-Methylpentane-2,4-dione                          | 10.87      |           |        |        |
| 2-Methylpentanoic acid                             | 4.782      |           |        |        |
| 3-Methylpentanoic acid                             | 4.766      |           |        |        |
| 4-Methylpentanoic acid                             | 4.845      |           |        |        |
| cis-3-Methyl-2-pentenoic acid                      | 5.15       |           |        |        |
| trans-3-Methyl-2-pentenoic acid                    | 5.13       |           |        |        |
| 4-Methyl-2-pentenoic acid                          | 4.70       |           |        |        |
| 4-Methyl-3-pentenoic acid                          | 4.60       |           |        |        |
| 6-Methyl-1,10-phenanthroline                       | 5.11(+1)   |           |        |        |
| (2-Methylphenoxy)acetic acid                       | 3.227      |           |        |        |
| (3-Methylphenoxy)acetic acid                       | 3.203      |           |        |        |
| (4-Methylphenoxy)acetic acid                       | 3.215      |           |        |        |
| (2-Methylphenyl)acetic acid (18°C)                 | 4.35       |           |        |        |
| (4-Methylphenyl)acetic acid                        | 4.370      |           |        |        |
| 5-Methyl-5-phenylbarbituric acid                   | 8.011(0)   |           |        |        |
| 3-(2-Methylphenyl)propanoic acid                   | 4.66       |           |        |        |
| 3-(3-Methylphenyl)propanoic acid                   | 4.677      |           |        |        |
| 3-(4-Methylphenyl)propanoic acid                   | 4.684      |           |        |        |
| 1-Methyl-2-phenylpyrrolidine                       | 8.80       |           |        |        |
| 5-Methyl-1-phenyl-1,2,3-triazole-4-carboxylic acid | 3.73       |           |        |        |
| Methylphosphinic acid                              | 3.08       |           |        |        |
| Methylphosphonic acid                              | 2.38       | 7.74      |        |        |
| 3-Methyl-o-phthalic acid                           | 3.18       |           |        |        |
| 4-Methyl-o-phthalic acid                           | 3.89       |           |        |        |
| N-Methylpiperazine ( $\mu = 0.1$ )                 | 4.94(+2)   | 9.09(+1)  |        |        |
| 2-Methylpiperazine                                 | 5.62(+2)   | 9.60(+1)  |        |        |
| N-Methylpiperidine                                 | 10.19(+1)  |           |        |        |
| 2-Methylpiperidine                                 | 10.95(+1)  |           |        |        |
| 3-Methylpiperidine                                 | 11.07(+1)  |           |        |        |
| 4-Methylpiperidine ( $\mu = 0.5$ )                 | 11.23(+1)  |           |        |        |
| 2-Methyl-1,2-propanediamine                        | 6.178(+2)  | 9.420(+1) |        |        |
| 2-Methyl-2-propanethiol                            | 11.2       |           |        |        |
| 2-Methylpropanoic acid                             | 4.853      |           |        |        |
| 2-Methyl-2-propylamine                             | 10.682(+1) |           |        |        |
| 2-Methyl-2-propylglutaric acid                     | 3.626      |           |        |        |
| 2-Methylpyridine                                   | 5.96(+1)   |           |        |        |
| 3-Methylpyridine                                   | 5.68(+1)   |           |        |        |
| 4-Methylpyridine                                   | 6.00(+1)   |           |        |        |
| Methyl 4-pyridinecarboxylate                       | 3.26(+1)   |           |        |        |
| 6-Methylpyridine-2-carboxylic acid                 | 5.83       |           |        |        |
| 2-Methylpyridine-1-oxide                           | 1.029(+1)  |           |        |        |
| 3-Methylpyridine-1-oxide                           | 10.921(+1) |           |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                       | $pK_1$    | $pK_2$  | $pK_3$ | $pK_4$ |
|---------------------------------------------------------------------------------|-----------|---------|--------|--------|
| 4-Methylpyridine-1-oxide                                                        | 1.258(+1) |         |        |        |
| O-Methylpyridoxal ( $\mu = 0.16$ )                                              | 4.74      |         |        |        |
| Methyl-2-pyridyl ketoxime                                                       | 9.97      |         |        |        |
| 1-Methyl-2-(3-pyridyl)pyrrolidine                                               | 3.41      | 7.94    |        |        |
| 1-Methylpyrrolidine                                                             | 10.46(+1) |         |        |        |
| 1-Methyl-3-pyrroline                                                            | 9.88(+1)  |         |        |        |
| 5-Methylquinoline                                                               | 4.62(+1)  |         |        |        |
| Methylsuccinic acid                                                             | 4.13      | 5.64    |        |        |
| Methylsulfonylacetic acid                                                       | 2.36      |         |        |        |
| 3-Methylsulfonylaniline                                                         | 2.68(+1)  |         |        |        |
| 4-Methylsulfonylaniline                                                         | 1.48(+1)  |         |        |        |
| 3-Methylsulfonylbenzoic acid                                                    | 3.52      |         |        |        |
| 4-Methylsulfonylbenzoic acid                                                    | 3.64      |         |        |        |
| 4-Methylsulfonyl-3,5-dimethylphenol                                             | 8.13      |         |        |        |
| 3-Methylsulfonylphenol                                                          | 9.33      |         |        |        |
| 4-Methylsulfonylphenol                                                          | 7.83      |         |        |        |
| 1-Methyl-1,2,3,4-tetrahydro-3-pyridinecarboxylic acid (arecaidine; isoguvacine) | 9.07      |         |        |        |
| 5-Methyl-1,2,3,4-tetrazole                                                      | 3.32      |         |        |        |
| 2-Methylthiazole ( $\mu = 0.1$ )                                                | 3.40(+1)  |         |        |        |
| 4-Methylthiazole ( $\mu = 0.1$ )                                                | 3.16(+1)  |         |        |        |
| 5-Methylthiazole ( $\mu = 0.1$ )                                                | 3.03(+1)  |         |        |        |
| Methylthioacetic acid                                                           | 3.72      |         |        |        |
| 4-Methylthioaniline                                                             | 4.40(+1)  |         |        |        |
| 2-Methylthioethylamine (30°C)                                                   | 9.18(+1)  |         |        |        |
| Methylthioglycolic acid                                                         | 7.68      |         |        |        |
| 3-(S-Methylthio)phenol                                                          | 9.53      |         |        |        |
| 4-(S-Methylthio)phenol                                                          | 9.53      |         |        |        |
| 2-Methylthiopyridine (20°C)                                                     | 3.59(+1)  |         |        |        |
| 3-Methylthiopyridine (20°C)                                                     | 4.42(+1)  |         |        |        |
| 4-Methylthiopyridine (20°C)                                                     | 5.94(+1)  |         |        |        |
| 5-Methylthio-1,2,3,4-tetrazole                                                  | 4.00(+1)  |         |        |        |
| O-Methylthreonine                                                               | 2.02(+1)  | 9.00(0) |        |        |
| O-Methyltyrosine                                                                | 2.21(+1)  | 9.35(0) |        |        |
| 1-Methylxanthine                                                                | 7.70      | 12.0    |        |        |
| 3-Methylxanthine                                                                | 8.10      | 11.3    |        |        |
| 7-Methylxanthine                                                                | 8.33      | ca 13   |        |        |
| 9-Methylxanthine                                                                | 6.25      |         |        |        |
| Morphine (20°C)                                                                 | 7.87(+1)  | 9.85(0) |        |        |
| Morpholine                                                                      | 8.492(+1) |         |        |        |
| 2-(N-Morpholino)ethanesulfonic acid (MES) (20°C)                                | 6.15      |         |        |        |
| 3-(N-Morpholino)-2-hydroxypropanesulfonic acid (37°C)                           | 6.75      |         |        |        |
| 3-(N-Morpholino)propanesulfonic acid (20°C)                                     | 7.20      |         |        |        |
| Murexide                                                                        | 0.0       | 9.20    | 10.50  |        |
| Myosmine                                                                        | 5.26      |         |        |        |
| 1-Naphthalenecarboxylic acid (1-naphthoic acid)                                 | 3.695     |         |        |        |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                               | $pK_1$    | $pK_2$    | $pK_3$ | $pK_4$ |
|---------------------------------------------------------|-----------|-----------|--------|--------|
| 2-Naphthalenecarboxylic acid                            | 4.161     |           |        |        |
| 1-Naphthol (20°C)                                       | 9.30      |           |        |        |
| 2-Naphthol (20°C)                                       | 9.57      |           |        |        |
| Naphthoquinone monoxime                                 | 8.01      |           |        |        |
| 1-Naphthylacetic acid                                   | 4.236     |           |        |        |
| 2-Naphthylacetic acid                                   | 4.256     |           |        |        |
| 1-Naphthylamine                                         | 3.92(+1)  |           |        |        |
| 2-Naphthylamine                                         | 4.11(+1)  |           |        |        |
| 1-Naphthylarsonic acid                                  | 3.66      | 8.66      |        |        |
| 1-Naphthysulfonic acid                                  | 0.57      |           |        |        |
| Narceine (15°C)                                         | 3.5(+1)   | 9.3       |        |        |
| Narcotine                                               | 6.18(+1)  |           |        |        |
| Nicotine                                                | 3.15(+1)  | 7.87(0)   |        |        |
| Nicotyrine                                              | 4.76(+1)  |           |        |        |
| Nitrilotriacetic acid (NTA) (20°C)                      | 1.65      | 2.94      | 10.33  |        |
| Nitroacetic acid                                        | 1.68      |           |        |        |
| 2-Nitroaniline                                          | -0.28(+1) |           |        |        |
| 3-Nitroaniline                                          | 2.46(+1)  |           |        |        |
| 4-Nitroaniline                                          | 1.01(+1)  |           |        |        |
| 2-Nitrobenzene-1,4-dicarboxylic acid                    | 1.73      |           |        |        |
| 3-Nitrobenzene-1,2-dicarboxylic acid                    | 1.88      |           |        |        |
| 4-Nitrobenzene-1,2-dicarboxylic acid                    | 2.11      |           |        |        |
| 2-Nitrobenzoic acid                                     | 2.18      |           |        |        |
| 3-Nitrobenzoic acid                                     | 3.46      |           |        |        |
| 4-Nitrobenzoic acid                                     | 3.441     |           |        |        |
| <i>trans</i> -2-Nitrocinnamic acid                      | 4.15      |           |        |        |
| <i>trans</i> -3-Nitrocinnamic acid                      | 4.12      |           |        |        |
| <i>trans</i> -4-Nitrocinnamic acid                      | 4.05      |           |        |        |
| Nitroethane                                             | 8.57      |           |        |        |
| 2-Nitrohydroquinone                                     | 7.63      | 10.06     |        |        |
| <i>N</i> -Nitroiminodiacetic acid                       | 2.21      | 3.33      |        |        |
| 3-Nitromesitol                                          | 8.984     |           |        |        |
| Nitromethane                                            | 10.12     |           |        |        |
| 1-Nitro-6,7-phenanthroline ( $\mu = 0.2$ )              | 3.23(+1)  |           |        |        |
| 5-Nitro-1,10-phenanthroline                             | 3.232(+1) |           |        |        |
| 6-Nitro-1,10-phenanthroline                             | 3.23(+1)  |           |        |        |
| 2-Nitrophenol                                           | 7.222     |           |        |        |
| 3-Nitrophenol                                           | 8.360     |           |        |        |
| 4-Nitrophenol                                           | 7.150     |           |        |        |
| (2-Nitrophenoxy)acetic acid                             | 2.896     |           |        |        |
| (3-Nitrophenoxy)acetic acid                             | 2.951     |           |        |        |
| (4-Nitrophenoxy)acetic acid                             | 2.893     |           |        |        |
| 2-Nitrophenylacetic acid                                | 4.00      |           |        |        |
| 3-Nitrophenylacetic acid                                | 3.97      |           |        |        |
| 4-Nitrophenylacetic acid                                | 3.85      |           |        |        |
| 2-Nitrophenylarsonic acid                               | 3.37      | 8.54      |        |        |
| 3-Nitrophenylarsonic acid                               | 3.41      | 7.80      |        |        |
| 4-Nitrophenylarsonic acid                               | 2.90      | 7.80      |        |        |
| 7-(4-Nitrophenylazo)-8-hydroxy-5-quinolinesulfonic acid | 3.14(0)   | 7.495(-1) |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                       | $pK_1$                    | $pK_2$     | $pK_3$   | $pK_4$ |
|-------------------------------------------------|---------------------------|------------|----------|--------|
| 3-Nitrophenylphosphonic acid                    | 1.30                      | 6.27       |          |        |
| 4-Nitrophenylphosphonic acid                    | 1.24                      | 6.23       |          |        |
| 3-(2'-Nitrophenyl)propanoic acid                | 4.504                     |            |          |        |
| 3-(4'-Nitrophenyl)propanoic acid                | 4.473                     |            |          |        |
| 3-Nitrophenylselenic acid                       | 4.07                      |            |          |        |
| 4-Nitrophenylselenic acid                       | 4.00                      |            |          |        |
| 1-Nitropropane                                  | 8.98                      |            |          |        |
| 2-Nitropropane                                  | 7.675                     |            |          |        |
| 2-Nitropropanoic acid                           | 3.79                      |            |          |        |
| 2-Nitropyridine ( $\mu = 0.02$ )                | -2.06(+1)                 |            |          |        |
| 3-Nitropyridine ( $\mu = 0.02$ )                | 0.79(+1)                  |            |          |        |
| 4-Nitropyridine ( $\mu = 0.02$ )                | 1.23(+1)                  |            |          |        |
| <i>N</i> -Nitrosoiminodiacetic acid             | 2.28                      | 3.38       |          |        |
| 4-Nitrosophenol                                 | 6.48                      |            |          |        |
| Nitrourea                                       | 4.15(+1)                  |            |          |        |
| 1,9-Nonanedioic acid (azelaic acid)             | 4.53                      | 5.40       |          |        |
| Nonanoic acid (pelargonic acid)                 | 4.95                      |            |          |        |
| <b>DL</b> -Norleucine                           | 2.335(+1)                 | 9.834(0)   |          |        |
| Novocaine                                       | 8.85(+1)                  |            |          |        |
| 2,2,3,3,4,4,5,5-Octafluoropentanoic acid        | 2.65                      |            |          |        |
| 1,8-Octanedioic acid (suberic acid)             | 4.512                     | 5.404      |          |        |
| Octanoic acid (caprylic acid)                   | 4.895                     |            |          |        |
| Octopine- <b>DD</b>                             | 1.35                      | 2.30       | 8.68     | 11.25  |
| Octopine- <b>LD</b>                             | 1.40                      | 2.30       | 8.72     | 11.34  |
| Octylamine                                      | 10.65(+1)                 |            |          |        |
| <b>L</b> -(+)-Ornithine                         | 1.94(+2)                  | 8.65(+1)   | 10.76(0) |        |
| Oxalic acid                                     | 1.271                     | 4.272      |          |        |
| 3,6-Oxaoctanedioic acid ( $\mu = 1.0$ )         | 3.055                     | 3.676      |          |        |
| Oxoacetic acid                                  | 3.46                      |            |          |        |
| 2-Oxabutanedioic acid (oxaloacetic acid)        | 2.56                      | 4.37       |          |        |
| 2-Oxobutanoic acid                              | 2.50                      |            |          |        |
| 5-Oxohexanoic acid (5-ketohexanoic acid) (18°C) | 4.662                     |            |          |        |
| 3-Oxo-1,5-pentanedioic acid                     | 3.10                      |            |          |        |
| 4-Oxopentanoic acid (levulinic acid)            | 4.59                      |            |          |        |
| 2-Oxopropanoic acid (pyruvic acid)              | 2.49                      |            |          |        |
| Oxytetracycline                                 | 3.10(+1)                  | 7.26       | 9.11     |        |
| Papaverine                                      | 5.90(+1)                  |            |          |        |
| Pentamethylenebis(thioacetic acid) (18°C)       | 3.485                     | 4.413      |          |        |
| 3,3-Pentamethylenepentanedioic acid             | 3.49                      | 6.96       |          |        |
| 1,5-Pentanediamine                              | 10.05(+2)                 | 10.916(+1) |          |        |
| 2,4-Pentanedione                                | 8.24(enol);<br>8.95(keto) |            |          |        |
| 1-Pentanoic acid (valeric acid)                 | 4.842                     |            |          |        |
| 2-Pentenoic acid                                | 4.70                      |            |          |        |
| 3-Pentenoic acid                                | 4.52                      |            |          |        |



**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                      | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$ |
|------------------------------------------------|-----------|-----------|-----------|--------|
| 4-Pentenoic acid                               | 4.677     |           |           |        |
| Pentylarsonic acid                             | 4.14      | 9.07      |           |        |
| <i>N</i> -Pentylveratramine                    | 7.28(+1)  |           |           |        |
| Perhydrodiphenic acid (20°C)                   | 4.96      | 6.68      |           |        |
| Perlolidine (18°C)                             | 4.01      | 11.39     |           |        |
| Peroxyacetic acid                              | 8.20      |           |           |        |
| 1,7-Phenanthroline                             | 4.30(+1)  |           |           |        |
| 1,10-Phenanthroline                            | 4.857(+1) |           |           |        |
| 6,7-Phenanthroline                             | 4.857(+1) |           |           |        |
| Phenazine                                      | 1.2(+1)   |           |           |        |
| Phenethylthioacetic acid                       | 3.795     |           |           |        |
| Phenol                                         | 9.99      |           |           |        |
| Phenol-3-phosphoric acid                       | 1.78      | 7.03      | 10.2      |        |
| Phenol-4-phosphoric acid                       | 1.99      | 7.25      | 9.9       |        |
| Phenolphthalein                                | 9.4       |           |           |        |
| 3-Phenolsulfonic acid                          | —         | 9.05(−1)  |           |        |
| Phenosulsulfonephthalein                       | 7.9       |           |           |        |
| Phenoxyactic acid                              | 3.171     |           |           |        |
| 2-Phenoxybenzoic acid                          | 3.53      |           |           |        |
| 3-Phenoxybenzoic acid                          | 3.95      |           |           |        |
| 4-Phenoxybenzoic acid                          | 4.52      |           |           |        |
| 5-Phenoxy-1,2,3,4-tetrazole                    | 3.49(+1)  |           |           |        |
| Phenylacetic acid                              | 4.312     |           |           |        |
| <b>L</b> -3-Phenyl- $\alpha$ -alanine          | 1.83(+1)  | 9.12(0)   |           |        |
| 3-Phenyl- $\alpha$ -alanine, methyl ester      | 7.05(+1)  |           |           |        |
| Phenylalanylarginine ( $\mu$ = 0.01)           | 2.66(+1)  | 7.57(0)   | 12.40(−1) |        |
| Phenylalanylglycine ( $\mu$ = 0.01)            | 3.10(+1)  | 7.71(0)   |           |        |
| 7-Phenylazo-8-hydroxy-5-quinolinesulfonic acid | 3.41(0)   | 7.850(−1) |           |        |
| 5-Phenylbarbituric acid                        | 2.544(+1) |           |           |        |
| 2-Phenyl-2-benzylsuccinic acid                 | 3.69      | 6.47      |           |        |
| 1-Phenylbiguanide                              | 2.13(+2)  | 10.76(+1) |           |        |
| 4-Phenylbutanoic acid                          | 4.757     |           |           |        |
| Phenylbutazone                                 | 4.5(+1)   |           |           |        |
| 2-Phenylenediamine                             | <2(+2)    | 4.47(+1)  |           |        |
| 3-Phenylenediamine                             | 2.65(+2)  | 4.88(+1)  |           |        |
| 4-Phenylenediamine                             | 3.29(+2)  | 6.08(+1)  |           |        |
| 2-Phenylethylamine                             | 9.83(+1)  |           |           |        |
| $\beta$ -Phenylethylboronic acid               | 10.0      |           |           |        |
| <b>DL</b> - $\alpha$ -Phenylglycine            | 1.83(+1)  | 4.39(0)   |           |        |
| Phenylguanidine                                | 10.77(+1) |           |           |        |
| Phenylhydrazine                                | 5.20(+1)  |           |           |        |
| 2-Phenyl-3-hydroxypropanoic acid               | 3.53      |           |           |        |
| 3-Phenyl-3-hydroxypropanoic acid               | 4.40      |           |           |        |
| Phenyliminodiacetic acid (20°C)                | 2.40      | 4.98      |           |        |
| Phenylmalonic acid                             | 2.58      | 5.03      |           |        |
| Phenylmethanethiol                             | 10.70     |           |           |        |
| 2-Phenyl-2-phenethylsuccinic acid (20°C)       | 3.74      | 6.52      |           |        |
| 2-Phenylphenol                                 | 9.55      |           |           |        |
| 3-Phenylphenol                                 | 9.63      |           |           |        |
| 4-Phenylphenol                                 | 9.55      |           |           |        |
| Phenylphosphinic acid (17°C)                   | 2.1       |           |           |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                     | $pK_1$     | $pK_2$    | $pK_3$   | $pK_4$ |
|-----------------------------------------------|------------|-----------|----------|--------|
| Phenylphosphonic acid                         | 1.83       | 7.07      |          |        |
| O-Phenylphosphorylserine                      | 2.13(+1)   | 8.79      |          |        |
| O-Phenylphosphorylserylglycine                | 3.18(+1)   | 6.95(0)   |          |        |
| O-Phenylphosphoryl-L-seryl-L-leucine          | 3.16(+1)   | 7.12(0)   |          |        |
| N-Phenylpiperazine ( $\mu = 0.1$ )            | 8.71(+1)   |           |          |        |
| 2-Phenylpropanoic acid                        | 4.38       |           |          |        |
| 3-Phenylpropanoic acid (35°C)                 | 4.664      |           |          |        |
| 3-Phenyl-1-propylamine                        | 10.39(+1)  |           |          |        |
| Phenylpropynoic acid (35°C)                   | 2.269      |           |          |        |
| Phenylselenic acid                            | 4.79       |           |          |        |
| Phenylselenoacetic acid ( $\mu = 0.1$ )       | 3.75       |           |          |        |
| $\beta$ -Phenylserine ( $\mu = 0.16$ )        | 8.79(0)    |           |          |        |
| Phenylsuccinic acid (20°C)                    | 3.78       | 5.55      |          |        |
| Phenylsulfenylacetic acid                     | 2.66       |           |          |        |
| Phenylsulfonylacetic acid                     | 2.44       |           |          |        |
| 5-Phenyl-1,2,3,4-tetrazole                    | 4.38(+1)   |           |          |        |
| 1-Phenyl-1,2,3-triazole-4-carboxylic acid     | 2.88       |           |          |        |
| 1-Phenyl-1,2,3-triazole-4,5-dicarboxylic acid | 2.13       | 4.93      |          |        |
| Phosphoramidic acid                           | 3.08       | 8.63      |          |        |
| O-Phosphorylethanolamine                      | 5.838(+1)  | 10.638(0) |          |        |
| O-Phosphorylserylglycine                      | 3.13       | 5.41      | 8.01     |        |
| O-Phosphoryl-L-seryl-L-leucine                | 3.11       | 5.47      | 8.26     |        |
| Phosphoserine                                 | 2.08       | 5.65      | 9.74     |        |
| Phthalamide                                   | 3.79(0)    |           |          |        |
| Phthalazine                                   | 3.47(+1)   |           |          |        |
| o-Phthalic acid                               | 2.950      | 5.408     |          |        |
| Phthalimide                                   | 9.90(0)    |           |          |        |
| Physostigmine                                 | 1.76(+1)   | 7.88(0)   |          |        |
| Picric acid (2,4,6-trinitrophenol) (18°C)     | 0.419      |           |          |        |
| Pilocarpine                                   | 1.3(+1)    | 6.85(0)   |          |        |
| Piperazine                                    | 5.333(+2)  | 9.781(+1) |          |        |
| 1,4-Piperazinebis(ethanesulfonic acid) (20°C) | 6.80       |           |          |        |
| Piperazine-2-carboxylic acid                  | 1.5        | 5.41      | 9.53     |        |
| Piperdine                                     | 11.123(+1) |           |          |        |
| 2-Piperidinecarboxylic acid                   | 2.12(+1)   | 10.75(0)  |          |        |
| 3-Piperidinecarboxylic acid                   | 3.35(+1)   | 10.64(0)  |          |        |
| 4-Piperidinecarboxylic acid                   | 3.73(+1)   | 10.72(0)  |          |        |
| 1-(2-Piperidinyl)-2-propanone (15°C)          | 9.45       |           |          |        |
| Piperine (15°C)                               | 1.98(+1)   |           |          |        |
| Proline                                       | 1.99(+1)   | 10.96(0)  |          |        |
| 1,2-Propanediamine                            | 6.607(+2)  | 9.702(+1) |          |        |
| 1,3-Propanediamine                            | 8.49(+2)   | 10.47(+1) |          |        |
| 1-Propanethiol                                | 10.86      |           |          |        |
| 1,2,3-Propanetriamine                         | 3.72(+3)   | 7.95(+2)  | 9.59(+1) |        |
| 1,2,3-Propanetricarboxylic acid               | 3.67       | 4.87      | 6.38     |        |
| Propanoic acid                                | 4.874      |           |          |        |
| Propenoic acid                                | 4.247      |           |          |        |

TABLE 8.8  $pK_a$  Values of Organic Materials in Water at 25°C (Continued)

| Substance                                                 | $pK_1$     | $pK_2$           | $pK_3$            | $pK_4$ |
|-----------------------------------------------------------|------------|------------------|-------------------|--------|
| <i>N</i> -Propionylglycine                                | 3.718(0)   |                  |                   |        |
| 2-Propoxybenzoic acid (20°C)                              | 4.24       |                  |                   |        |
| 3-Propoxybenzoic acid (20°C)                              | 4.20       |                  |                   |        |
| 4-Propoxybenzoic acid (20°C)                              | 4.78       |                  |                   |        |
| <i>N</i> -Propylalanine                                   | 2.21(+1)   | 10.19(0)         |                   |        |
| Propylamine                                               | 10.568(+1) |                  |                   |        |
| Propylarsonic acid (18°C)                                 | 4.21       | 9.09             |                   |        |
| Propylenimine                                             | 8.18(+1)   |                  |                   |        |
| <i>N</i> -Propylglycine ( $\mu = 0.1$ )                   | 2.38(+1)   | 10.03(0)         |                   |        |
| <i>L</i> -Propylglycine                                   | 3.19(+1)   | 8.97(0)          |                   |        |
| Propylmalonic acid                                        | 2.97       | 5.84             |                   |        |
| Propylphosphinic acid                                     | 3.46       |                  |                   |        |
| Propylphosphonic acid                                     | 2.49       | 8.18             |                   |        |
| 2-Propylpyridine                                          | 6.30(+1)   |                  |                   |        |
| <i>N</i> -Propylveratramine                               | 7.20(+1)   |                  |                   |        |
| 2-Propynoic acid                                          | 1.887      |                  |                   |        |
| Pseudoecgonine                                            | 9.70       |                  |                   |        |
| Pseudoisocyanine ( $\mu = 0.2$ )                          | 4.59(+2)   |                  |                   |        |
| Pseudotropine                                             | 9.86(+1)   |                  |                   |        |
| Pteroylglutamic acid                                      | 8.26       |                  |                   |        |
| Purine                                                    | 2.52(+1)   | 8.92(0)          |                   |        |
| Pyrazine                                                  | 0.6(+1)    |                  |                   |        |
| Pyrazinecarboxamide                                       | 0.5(+1)    |                  |                   |        |
| Pyrazole                                                  | 2.61(+1)   |                  |                   |        |
| Pyridazine                                                | 2.33(+1)   |                  |                   |        |
| Pyridine                                                  | 5.17(+1)   |                  |                   |        |
| Pyridine- $d_5$                                           | 5.83(+1)   |                  |                   |        |
| 2-Pyridinealdoxime                                        | 3.56(+1)   | 10.17(0)         |                   |        |
| 3-Pyridinealdoxime                                        | 4.07(+1)   | 10.39(0)         |                   |        |
| 4-Pyridinealdoxime                                        | 4.73(+1)   | 10.03(0)         |                   |        |
| 2-Pyridinecarbaldehyde                                    | 3.84(+1)   |                  |                   |        |
| 3-Pyridinecarbaldehyde                                    | 3.80(+1)   |                  |                   |        |
| 4-Pyridinecarbaldehyde                                    | 4.74(+1)   |                  |                   |        |
| 3-Pyridinecarbamide (nicotin-<br>amide)                   | 3.33(+1)   |                  |                   |        |
| 3-Pyridinecarbonitrile                                    | 1.35(+1)   |                  |                   |        |
| Pyridine-2-carboxylic acid (picol-<br>inic acid)          | 1.01(+1)   | 5.29(0)          |                   |        |
| Pyridine-3-carboxylic acid (nico-<br>tinic acid)          | 2.07(+1)   | 4.75(0)          |                   |        |
| Pyridine-4-carboxylic acid (isoni-<br>cotic acid)         | 1.84(+1)   | 4.86(0)          |                   |        |
| Pyridine-2,3-dicarboxylic acid                            | 2.36(+1)   | 7.08(0)          |                   |        |
| Pyridine-2,4-dicarboxylic acid                            | 2.23(+1)   | 7.02(0)          |                   |        |
| Pyridine-2,6-dicarboxylic acid                            | 2.16(+1)   | 6.92(0)          |                   |        |
| Pyridine-1-oxide                                          | 0.688(+1)  |                  |                   |        |
| Pyridoxal                                                 | 4.20(+1)   | 8.66(ring<br>OH) |                   |        |
| Pyridoxal-5-phosphate ( $\mu = 0.15$ )                    | <2.5       | 4.14             | 6.20              | 8.69   |
| Pyridoxamine ( $\mu = 0.1$ )                              | 3.37(+2)   | 8.01(+1)         | 10.13(ring<br>OH) |        |
| Pyridoxamine-5-phosphate ( $\mu =$<br>0.15; $pK_5$ 10.92) | 2.5        | 3.69             | 5.76              | 8.61   |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                  | $pK_1$     | $pK_2$           | $pK_3$    | $pK_4$ |
|------------------------------------------------------------|------------|------------------|-----------|--------|
| Pyridoxine (vitamin B <sub>6</sub> ) (18°C)                | 5.00(+1)   | 8.96(ring<br>OH) |           |        |
| 3-(2'-Pyridyl)alanine                                      | 1.37(+2)   | 4.02(+1)         | 9.22(0)   |        |
| 3-(3'-Pyridyl)alanine                                      | 1.77(+2)   | 4.64(+1)         | 9.10(0)   |        |
| 2-(2'-Pyridyl)benzimidazole ( $\mu = 0.16$ )               | 5.58(+1)   |                  |           |        |
| 2-(2'-Pyridyl)imidazole ( $\mu = 0.005$ )                  | 8.98(+1)   |                  |           |        |
| 4-(2'-Pyridyl)imidazole ( $\mu = 0.1$ )                    | 5.49(+1)   |                  |           |        |
| Pyrimidine                                                 | 1.30(+1)   |                  |           |        |
| 2,4(1 <i>H</i> ,3 <i>H</i> )-Pyrimidinedione (uracil)      | 0.6(+1)    | 9.46(0)          |           |        |
| 2,4,5,6(1 <i>H</i> ,3 <i>H</i> )-Pyrimidinetetrone-5-oxime | 4.57(0)    |                  |           |        |
| Pyrocatecholsulfonephthaleine                              | 7.82       | 9.76             | 11.73     |        |
| Pyroxilidine                                               | 11.11(+1)  |                  |           |        |
| Pyrrole-1-carboxylic acid                                  | 4.45       |                  |           |        |
| Pyrrole-2-carboxylic acid                                  | 4.45       |                  |           |        |
| Pyrrole-3-carboxylic acid                                  | 4.453      |                  |           |        |
| Pyrrolidine                                                | 11.305(+1) |                  |           |        |
| Pyrrolidine-2-carboxylic acid (proline)                    | 1.952(+1)  | 10.640(0)        |           |        |
| 2-[2-( <i>N</i> -Pyrrolidinyl)ethyl]pyridine               | 3.60(+2)   | 9.39(+1)         |           |        |
| 3-[2-( <i>N</i> -Pyrrolidinyl)ethyl]pyridine               | 4.28(+2)   | 9.28(+1)         |           |        |
| 4-[2-( <i>N</i> -Pyrrolidinyl)ethyl]pyridine               | 4.65(+2)   | 9.27(+1)         |           |        |
| 2-(1-Pyrrolidinylmethyl)pyridine                           | 2.54(+1)   | 8.56(+1)         |           |        |
| 3-(1-Pyrrolidinylmethyl)pyridine                           | 3.14(+2)   | 8.36(+1)         |           |        |
| 4-(1-Pyrrolidinylmethyl)pyridine                           | 3.38(+2)   | 8.16(+1)         |           |        |
| 3-Pyrroline                                                | -0.27(+1)  |                  |           |        |
| Quinidine                                                  | 4.0(+1)    | 8.54(0)          |           |        |
| Quinine                                                    | 4.11(+1)   | 8.52(0)          |           |        |
| Quinoline                                                  | 4.80(+1)   |                  |           |        |
| Quinoxaline                                                | 0.72(+1)   |                  |           |        |
| <b>D</b> -Raffinose                                        | 12.74      |                  |           |        |
| Riboflavin (vitamin B <sub>2</sub> ) ( $\mu = 0.01$ )      | ca -0.2    | 9.69             |           |        |
| $\alpha$ - <b>D</b> -Ribofuranose                          | 12.11      |                  |           |        |
| <b>D</b> -Ribose-5'-phosphonic acid                        | —          | 6.70(-1)         | 13.05(-2) |        |
| <b>D</b> -Saccharic acid                                   | 5.00(0)    |                  |           |        |
| Saccharin ( <i>o</i> -benzoic sulfimide)                   | 2.32       |                  |           |        |
| Sarcosine                                                  | 2.12(+1)   | 10.20(0)         |           |        |
| Sarcosine amide                                            | 8.35(+1)   |                  |           |        |
| Sarcosine dimethylamide                                    | 8.86(+1)   |                  |           |        |
| Sarcosine methylamide                                      | 8.28(+1)   |                  |           |        |
| Sarcosylglycine ( $\mu = 0.16$ )                           | 3.15(+1)   | 8.56(0)          |           |        |
| Sarcosylleucine                                            | 3.15(+1)   | 8.67(0)          |           |        |
| Sarcosylsarcosine                                          | 2.92(+1)   | 9.15(0)          |           |        |
| Sarcosylserine                                             | 3.17(+1)   | 8.63(0)          |           |        |
| 3-Selenosemicarbazide ( $\mu = 0.1$ )                      | 0.8(+1)    |                  |           |        |
| Semicarbazide ( $\mu = 0.1$ )                              | 3.53(+1)   |                  |           |        |
| <b>L</b> -Serine                                           | 2.21(+1)   | 9.15(0)          | 13.6      |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                | $pK_1$    | $pK_2$    | $pK_3$    | $pK_4$   |
|----------------------------------------------------------|-----------|-----------|-----------|----------|
| Serine, methyl ester ( $\mu = 0.1$ )                     | 7.03(+1)  |           |           |          |
| Serylglycine ( $\mu = 0.15$ )                            | 2.10(+1)  | 7.33(0)   |           |          |
| L-Seryl-L-leucine                                        | 3.08(+1)  | 7.45(0)   |           |          |
| Solanine                                                 | 7.34(+1)  |           |           |          |
| D-Sorbitol (17.5°C)                                      | 13.60     |           |           |          |
| L-(−)-Sorbose (18°C)                                     | 11.55     |           |           |          |
| Sparteine                                                | 4.49(+1)  | 11.76(0)  |           |          |
| Spinaceamine ( $\mu = 0.1$ )                             | 4.895(+2) | 8.90(+1)  |           |          |
| Spinacine                                                | 1.649(+2) | 4.936(+1) | 8.663(0)  |          |
| L-Strychnine (15°C)                                      | 2.50      | 8.20      |           |          |
| Succinamic acid (succinic acid monoamide)                | 4.39(0)   |           |           |          |
| Succinic acid                                            | 4.207     | 5.635     |           |          |
| DL-Succinimide                                           | 9.623     |           |           |          |
| $\beta$ -(4'-Sulfaminophenyl)alanine                     | 1.99(+1)  | 8.64(0)   | 10.26(−1) |          |
| 3-Sulfamylbenzoic acid                                   | 3.54      |           |           |          |
| 4-Sulfamylbenzoic acid                                   | 3.47      |           |           |          |
| 4-Sulfamylphenylphosphoric acid                          | 1.42      | 6.38      | 10.0      |          |
| Sulfanilamide                                            | 10.43(+1) |           |           |          |
| Sulfoacetic acid                                         | —         | 4.0       |           |          |
| 3-Sulfobenzoic acid                                      | —         | 3.78      |           |          |
| 4-Sulfobenzoic acid                                      | —         | 3.72      |           |          |
| 3-Sulfophenol                                            | 0.39      | 9.07      |           |          |
| 4-Sulfophenol                                            | 0.58      | 8.70      |           |          |
| 2-Sulfopropanoic acid                                    | 1.99      |           |           |          |
| 5-Sulfosalicyclic acid                                   | 2.49      | 12.00     |           |          |
| Sylvic acid                                              | 7.62      |           |           |          |
| D-Tartaric acid                                          | 3.036     | 4.366     |           |          |
| meso-Tartaric acid                                       | 3.22      | 4.81      |           |          |
| Tetracycline ( $\mu = 0.005$ )                           | 3.30(+1)  | 7.68      | 9.69      |          |
| Tetradehydrohimbine                                      | 10.59(+1) |           |           |          |
| Tetraethylenepentamine [ $\mu = 0.1$ ; $pK_s$ 9.67(+1)]  | 2.98(+5)  | 4.72(+4)  | 8.08(+3)  | 9.10(+2) |
| 1,4,5,6-Tetrahydro-1,2-dimethylpyridine                  | 11.38(+1) |           |           |          |
| 1,4,5,6-Tetrahydro-2-methylpyridine                      | 9.53(+1)  |           |           |          |
| cis-Tetrahydronaphthalene-2,3-dicarboxylic acid (20°C)   | 3.98      | 6.47      |           |          |
| trans-Tetrahydronaphthalene-2,3-dicarboxylic acid (20°C) | 4.00      | 5.70      |           |          |
| 5,6,7,8-Tetrahydro-1-naphthol                            | 10.28     |           |           |          |
| 5,6,7,8-Tetrahydro-2-naphthol                            | 10.48     |           |           |          |
| Tetrahydroserpentine                                     | 10.55(+1) |           |           |          |
| 2,3,5,6-Tetramethylbenzoic acid                          | 3.415     |           |           |          |
| Tetramethylenebis(thioacetic acid) (18°C)                | 3.463     | 4.423     |           |          |
| Tetramethylenediamine                                    | 9.22(+2)  | 10.75(+1) |           |          |
| N,N,N',N'-Tetramethylethylenediamine                     | 2.20(+2)  | 6.35(+1)  |           |          |
| 2,3,5,6-Tetramethyl-4-methylaminopyridine                | 0.07(+1)  |           |           |          |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                     | $pK_1$    | $pK_2$ | $pK_3$ | $pK_4$ |
|-----------------------------------------------|-----------|--------|--------|--------|
| 2,2,6,6-Tetramethylpiperidine ( $\mu = 0.5$ ) | 1.24(+1)  |        |        |        |
| 2,3,5,6-Tetramethylpyridine (20°C)            | 7.90(+1)  |        |        |        |
| Tetramethylsuccinic acid                      | 3.50      | 7.28   |        |        |
| 1,2,3,4-Tetrazole                             | 4.90      |        |        |        |
| Thebaine                                      | 7.95(+1)  |        |        |        |
| 2-Thenoyltrifluoroacetone                     | 5.70(0)   |        |        |        |
| Theobromine                                   | 0.68(+1)  | 7.89   |        |        |
| Theophylline                                  | <1(+1)    | 8.80   |        |        |
| Thiazoline                                    | 2.53(+1)  |        |        |        |
| Thioacetic acid                               | 3.33      |        |        |        |
| <i>o</i> -Thiocresol                          | 6.64      |        |        |        |
| <i>m</i> -Thiocresol                          | 6.58      |        |        |        |
| <i>p</i> -Thiocresol                          | 6.52      |        |        |        |
| Thiocyanatoacetic acid                        | 2.58      |        |        |        |
| 2,2'-Thiodiacetic acid                        | 3.32      | 4.29   |        |        |
| 4,4'-Thiodibutanoic acid (18°C)               | 4.351     | 5.275  |        |        |
| 3,3'-Thiodipropanoic acid (18°C)              | 4.085     | 5.075  |        |        |
| 3-Thio-S-methylcarbazine ( $\mu = 0.1$ )      | 7.563(+1) |        |        |        |
| 1-Thionylcarboxylic acid                      | 3.53      |        |        |        |
| 2-Thionylcarboxylic acid                      | 4.10      |        |        |        |
| 2-Thiophenecarboxylic acid (30°C)             | 3.529     |        |        |        |
| 3-Thiophenecarboxylic acid (3-thenoic acid)   | 4.10      |        |        |        |
| Thiophenol                                    | 6.50      |        |        |        |
| 3-Thiosemicarbazide ( $\mu = 0.1$ )           | 1.5(+1)   |        |        |        |
| 3-Thiosemicarbazide-1,1-diacetic acid (30°C)  | 2.94      | 4.07   |        |        |
| Thiourea                                      | 2.03(+1)  |        |        |        |
| Thorin                                        | 3.7       | 8.3    | 11.8   |        |
| Thymidine                                     | 9.79      | 12.85  |        |        |
| <i>p</i> -Toluenesulfinic acid                | 1.7       |        |        |        |
| Toluhydroquinone                              | 10.03     | 11.62  |        |        |
| <i>o</i> -Toluidine                           | 4.45(+1)  |        |        |        |
| <i>m</i> -Toluidine                           | 4.71(+1)  |        |        |        |
| <i>p</i> -Toluidine                           | 5.08(+1)  |        |        |        |
| <i>o</i> -Tolylacetic acid (18°C)             | 4.36      |        |        |        |
| <i>p</i> -Tolylacetic acid (18°C)             | 4.36      |        |        |        |
| <i>o</i> -Tolylarsonic acid                   | 3.82      | 8.85   |        |        |
| <i>m</i> -Tolylarsonic acid                   | 3.82      | 8.60   |        |        |
| <i>p</i> -Tolylarsonic acid                   | 3.70      | 8.68   |        |        |
| <i>o</i> -Tolylphosphonic acid                | 2.10      | 7.68   |        |        |
| <i>m</i> -Tolylphosphonic acid                | 1.88      | 7.44   |        |        |
| <i>p</i> -Tolylphosphonic acid                | 1.84      | 7.33   |        |        |
| 3-Tolylselenic acid                           | 4.80      |        |        |        |
| 4-Tolylselenic acid                           | 4.88      |        |        |        |
| Triacetylmethane                              | 5.81      |        |        |        |
| Triallylamine                                 | 8.31(+1)  |        |        |        |
| 1,3,5-Triazine-2,4,6-triol                    | 7.20      | 11.10  |        |        |
| 1 <i>H</i> -1,2,3-Triazole                    | —         | 9.26   |        |        |
| 1 <i>H</i> -1,2,4-Triazole                    | 2.386(+1) | 9.972  |        |        |
| 1,2,3-Triazole-4-carboxylic acid              | 3.22      | 8.73   |        |        |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                       | $pK_1$    | $pK_2$    | $pK_3$   | $pK_4$   |
|---------------------------------------------------------------------------------|-----------|-----------|----------|----------|
| 1,2,3-Triazole-4,5-dicarboxylic acid                                            | 1.86      | 5.90      | 9.30     |          |
| 1,2,4-Triazolidine-3,5-dione (urazole)                                          | 5.80      |           |          |          |
| Tribromoacetic acid                                                             | −0.147    |           |          |          |
| 2,4,6-Tribromobenzoic acid                                                      | 1.41      |           |          |          |
| Trichloroacetic acid                                                            | 0.52      |           |          |          |
| Trichloroacrylic acid                                                           | 1.15      |           |          |          |
| 3,3,3-Trichlorolactic acid                                                      | 2.34      |           |          |          |
| Trichloromethylphosphonic acid                                                  | 1.63      | 4.81      |          |          |
| 2,4,5-Trichlorophenol                                                           | 7.37      |           |          |          |
| 3,4,5-Trichlorophenol                                                           | 7.839     |           |          |          |
| Tricine (20°C)                                                                  | 8.15      |           |          |          |
| Triethanolamine                                                                 | 7.76(+1)  |           |          |          |
| Triethylamine                                                                   | 10.72(+1) |           |          |          |
| Triethylenediamine                                                              | 4.18(+2)  | 8.19(+1)  |          |          |
| Triethylenetetramine (20°C)                                                     | 3.32(+4)  | 6.67(+3)  | 9.20(+2) | 9.92(+1) |
| Triethylsuccinic acid                                                           | 2.74      |           |          |          |
| Trifluoroacetic acid                                                            | 0.50      |           |          |          |
| Trifluoroacrylic acid                                                           | 1.79      |           |          |          |
| 4,4,4-Trifluoro-2-aminobutanoic acid                                            | 1.600(+1) | 8.169(0)  |          |          |
| 4,4,4-Trifluoro-3-aminobutanoic acid                                            | 2.756(+1) | 5.822(0)  |          |          |
| 4,4,4-Trifluorobutanoic acid                                                    | 4.16      |           |          |          |
| $\alpha,\alpha,\alpha$ -Trifluoro- <i>m</i> -cresol                             | 8.950     |           |          |          |
| 4,4,4-Trifluorocrotonic acid                                                    | 3.15      |           |          |          |
| 5,5,5-Trifluoroleucine                                                          | 2.045(+1) | 8.942(0)  |          |          |
| 3-(Trifluoromethyl)aniline                                                      | 3.5(+1)   |           |          |          |
| 4-(Trifluoromethyl)aniline                                                      | 2.6(+1)   |           |          |          |
| 3-Trifluoromethylphenol                                                         | 8.950     |           |          |          |
| 5-Trifluoromethyl-1,2,3,4-tetrazole                                             | 1.70      |           |          |          |
| 6,6,6-Trifluoronorleucine                                                       | 2.164(+1) | 9.463(0)  |          |          |
| 5,5,5-Trifluoronorvaline                                                        | 2.042(+1) | 8.916(0)  |          |          |
| 5,5,5-Trifluoropentanoic acid                                                   | 4.50      |           |          |          |
| 3,3,3-Trifluoropropanoic acid                                                   | 3.06      |           |          |          |
| 4,4,4-Trifluorothreonine                                                        | 1.554(+1) | 7.822(0)  |          |          |
| 4,4,4-Trifluorovaline                                                           | 1.537(+1) | 8.098(0)  |          |          |
| 1,2,3-Trihydroxybenzene (pyrogallol)                                            | 9.03(0)   | 11.63(−1) |          |          |
| 1,3,5-Trihydroxybenzene (phloroglucinol)                                        | 8.45(0)   | 8.88(−1)  |          |          |
| 2,4,6-Trihydroxybenzoic acid                                                    | 1.68(0)   |           |          |          |
| 3,4,5-Trihydroxybenzoic acid                                                    | 4.19(0)   | 8.85(−1)  |          |          |
| 3,4,5-Trihydroxycyclohex-1-ene-1-carboxylic acid [ <b>D</b> -(−)-shikimic acid] | 4.15      |           |          |          |
| 2,4,6-Tri(hydroxymethyl)phenol                                                  | 9.56      |           |          |          |
| Triisobutylamine                                                                | 10.42(+1) |           |          |          |
| Trimethylamine                                                                  | 9.80(+1)  |           |          |          |
| 3-(Trimethylamino)phenol                                                        | 8.06      |           |          |          |
| 4-(Trimethylamino)phenol                                                        | 8.35      |           |          |          |

**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                                                      | $pK_1$     | $pK_2$  | $pK_3$   | $pK_4$    |
|--------------------------------------------------------------------------------|------------|---------|----------|-----------|
| 2,4,6-Trimethylaniline                                                         | 4.38(+1)   |         |          |           |
| 2,4,6-Trimethylbenzoic acid                                                    | 3.448      |         |          |           |
| Trimethylenebis(thioacetic acid)<br>(18°C)                                     | 3.435      | 5.383   |          |           |
| 2,3,4-Trimethylphenol                                                          | 10.59      |         |          |           |
| 2,4,5-Trimethylphenol                                                          | 10.57      |         |          |           |
| 2,4,6-Trimethylphenol                                                          | 10.88      |         |          |           |
| 3,4,5-Trimethylphenol                                                          | 10.25      |         |          |           |
| 2,3,6-Trimethylpyridine ( $\mu = 0.5$ )                                        | 7.60(+1)   |         |          |           |
| 2,4,6-Trimethylpyridine                                                        | 7.43(+1)   |         |          |           |
| 2,4,6-Trimethylpyridine-1-oxide                                                | 1.990(+1)  |         |          |           |
| 3-(Trimethylsilyl)benzoic acid                                                 | 4.089      |         |          |           |
| 4-(Trimethylsilyl)benzoic acid                                                 | 4.192      |         |          |           |
| 2,4,5-Trimethylthiazole ( $\mu = 0.1$ )                                        | 4.55       |         |          |           |
| 2,4,6-Trinitroaniline (picramide)                                              | -10.23(+1) |         |          |           |
| 2,4,6-Trinitrobenzene acid                                                     | 0.654      |         |          |           |
| 2,2,2-Trinitroethanol                                                          | 2.36       |         |          |           |
| Trinitromethane (20°C)                                                         | 0.17       |         |          |           |
| Triphenylacetic acid                                                           | 3.96       |         |          |           |
| Tripropylamine                                                                 | 10.66(+1)  |         |          |           |
| Tris(2-hydroxyethyl)amine                                                      | 7.762(+1)  |         |          |           |
| Tri(hydroxymethyl)aminomethane<br>(TRIS)                                       | 8.08(+1)   |         |          |           |
| 2-[Tris(hydroxymethyl)methyl<br>amino]-1-ethanesulfonic acid<br>(TES)          | 7.50       |         |          |           |
| 3-[Tris(hydroxymethyl)methyl<br>amino]-1-propanesulfonic acid<br>(TAPS) (20°C) | 8.4        |         |          |           |
| N-[Tris(hydroxymethyl)methyl]-<br>glycine (tricine)                            | 2.023(+1)  | 8.135   |          |           |
| Tris(trimethylsilyl)amine                                                      | 4.70(+1)   |         |          |           |
| Trithiocarbonic acid (20°C)                                                    | 2.64       |         |          |           |
| Tropacocaine (15°C)                                                            | 9.88(+1)   |         |          |           |
| 3-Tropanol (tropine)                                                           | 10.33(+1)  |         |          |           |
| Trypsin ( $\mu = 0.1$ )                                                        | 6.25       |         |          |           |
| L-Tryptophan                                                                   | 2.38(+1)   | 9.39(0) |          |           |
| DL-Tyrosine                                                                    | 2.18(+1)   | 9.11(0) | 10.6(OH) |           |
| Tyrosine amide                                                                 | 7.48       | 9.89    |          |           |
| Tyrosine, ethyl ester                                                          | 7.33       | 9.80    |          |           |
| Tyrosylarginine ( $\mu = 0.01$ )                                               | 2.65(+1)   | 7.39(0) | 9.36(-1) | 11.62(-2) |
| Tyrosyltyrosine                                                                | 3.52(+1)   | 7.68(0) | 9.80(-1) | 10.26(-2) |
| $\alpha$ -Ureidobutanoic acid                                                  | 3.886(0)   |         |          |           |
| $\gamma$ -Ureidobutanoic acid                                                  | 4.683(0)   |         |          |           |
| $\beta$ -Ureidopropanoic acid                                                  | 4.487(0)   |         |          |           |
| Uric acid                                                                      | 5.40       | 5.53    |          |           |
| Uridine                                                                        | 9.30       |         |          |           |
| Uridine-5'-diphosphoric acid                                                   | 7.16       |         |          |           |
| Uridine-5'-phosphoric acid (5'-uri-<br>dylic acid)                             | 6.63       |         |          |           |
| Uridine-5'-triphosphoric acid                                                  | 7.58       |         |          |           |



**TABLE 8.8**  $pK_a$  Values of Organic Materials in Water at 25°C (*Continued*)

| Substance                                               | $pK_1$    | $pK_2$   | $pK_3$    | $pK_4$   |
|---------------------------------------------------------|-----------|----------|-----------|----------|
| <b>DL</b> -Valine                                       | 2.32(+1)  | 9.61(0)  |           |          |
| <b>L</b> -Valine                                        | 2.296(+1) | 9.79(0)  |           |          |
| Valine amide ( $\mu = 0.2$ )                            | 8.00      |          |           |          |
| <b>L</b> -Valine, methyl ester                          | 7.49(+1)  |          |           |          |
| <b>L</b> -Valylglycine                                  | 3.23(+1)  | 8.00(0)  |           |          |
| Vetramine                                               | 7.49(+1)  |          |           |          |
| Veratrine                                               | 8.85(+1)  |          |           |          |
| Vinylmethylamine                                        | 9.69(+1)  |          |           |          |
| 2-Vinylpyridine                                         | 4.98(+1)  |          |           |          |
| 4-Vinylpyridine                                         | 5.62(+1)  |          |           |          |
| Vitamin B <sub>12</sub>                                 | 7.64(+1)  |          |           |          |
| Xanthine (40°C)                                         | 0.68(+1)  |          |           |          |
| Xanthosine                                              | <2.5(+1)  | 5.67(0)  | 12.00(−1) |          |
| Xylenol Orange [ $pK_5$ 10.46(−4);<br>$pK_6$ 12.28(−5)] | —         | 2.58(−1) | 3.23(−2)  | 6.37(−3) |
| <b>D</b> -(+)-Xylose                                    | 12.15(0)  |          |           |          |
| Zincon                                                  | —         | 4        | 7.85      | 15       |

**TABLE 8.9** Selected Equilibrium Constants in Aqueous Solution at Various Temperatures

**Abbreviations Used in the Table**

- (+ 1), protonated cation
- (0), neutral molecule
- (− 1), singly ionized anion
- (− 2), doubly ionized anion
- $pK_{\text{auto}}$ , negative logarithm (base 10) of autoprotolysis constant
- $pK_{\text{sp}}$ , negative logarithm (base 10) of solubility product

| Substance                                           | Temperature, °C |       |        |        |        |        |        |                         |        |       |
|-----------------------------------------------------|-----------------|-------|--------|--------|--------|--------|--------|-------------------------|--------|-------|
|                                                     | 0               | 5     | 10     | 15     | 20     | 25     | 30     | 35                      | 40     | 50    |
| Acetic acid (0)                                     | 4.780           | 4.770 | 4.762  | 4.758  | 4.757  | 4.756  | 4.757  | 4.762                   | 4.769  | 4.787 |
| DL-N-Acetylalanine (+ 1)                            |                 | 3.699 | 3.699  | 3.703  | 3.708  | 3.715  | 3.725  | 3.733                   | 3.745  | 3.774 |
| β-Acetylaminopropionic (+ 1)                        |                 | 4.479 | 4.465  | 4.465  | 4.449  | 4.445  | 4.444  | 4.443                   | 4.445  | 4.457 |
| N-Acetyl glycine (+ 1)                              |                 | 3.682 | 3.676  | 3.673  | 3.667  | 3.670  | 3.673  | 3.678                   | 3.685  | 3.706 |
| α-Alanine                                           |                 |       |        |        |        |        |        |                         |        |       |
| (+ 1)                                               | 2.42            |       | 2.39   |        | 2.35   | 2.34   | 2.33   | 2.33                    | 2.33   | 2.33  |
| (0)                                                 | 10.59           |       | 10.29  |        | 10.01  | 9.87   | 9.74   | 9.62                    | 9.49   | 9.26  |
| 2-Aminobenzenesulfonic acid (0),<br>pK <sub>2</sub> | 2.633           | 2.591 | 2.556  | 2.521  | 2.448  | 2.459  | 2.431  | 2.404                   | 2.380  | 2.338 |
| 3-Aminobenzenesulfonic acid (0),<br>pK <sub>2</sub> | 4.075           | 4.002 | 3.932  | 3.865  | 3.799  | 3.738  | 3.679  | 3.622                   | 3.567  | 3.464 |
| 4-Aminobenzenesulfonic acid (0),<br>pK <sub>2</sub> | 3.521           | 3.457 | 3.398  | 3.338  | 3.283  | 3.227  | 3.176  | 3.126                   | 3.079  | 2.989 |
| 3-Aminobenzoic acid (0)                             |                 |       |        |        | 4.90   | 4.79   | 4.75   |                         | 4.68   | 4.60  |
| 4-Aminobenzoic acid (0)                             |                 |       |        |        | 4.95   | 4.85   | 4.90   |                         | 4.95   | 5.10  |
| 2-Aminobutyric acid                                 |                 |       |        |        |        |        |        |                         |        |       |
| (+ 1)                                               |                 |       | 2.334  |        |        | 2.286  |        | 2.289 <sup>37.5°C</sup> |        | 2.297 |
| (0)                                                 |                 |       | 10.530 |        |        | 9.380  |        | 9.518 <sup>37.5°C</sup> |        | 9.234 |
| 4-Aminobutyric acid                                 |                 |       |        |        |        |        |        |                         |        |       |
| (+ 1)                                               |                 |       | 4.057  | 4.046  | 4.038  | 4.031  | 4.027  | 4.025                   | 4.027  | 4.032 |
| (0)                                                 |                 |       | 11.026 | 10.867 | 10.706 | 10.556 | 10.409 | 10.269                  | 10.114 | 9.874 |
| 2-Aminoethylsulfonic acid (0)                       |                 |       | 9.452  | 9.316  | 9.186  | 9.061  | 8.940  | 8.824                   | 8.712  | 9.499 |

**TABLE 8.9** Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*Continued*)

| Substance                               | Temperature, °C       |        |                          |                          |       |        |       |                         |       |       |
|-----------------------------------------|-----------------------|--------|--------------------------|--------------------------|-------|--------|-------|-------------------------|-------|-------|
|                                         | 0                     | 5      | 10                       | 15                       | 20    | 25     | 30    | 35                      | 40    | 50    |
| 2-Amino-3-methylpentanoic acid<br>(+ 1) | 2.365 <sup>1°C</sup>  |        | 2.338 <sup>12.5°C</sup>  |                          |       | 2.320  |       | 2.317 <sup>37.5°C</sup> |       | 2.332 |
| (0)                                     | 10.460 <sup>1°C</sup> |        | 10.100 <sup>12.5°C</sup> |                          |       | 9.758  |       | 9.439 <sup>37.5°C</sup> |       | 9.157 |
| 2-Amino-2-methyl-<br>1,3-propanediol    | 9.612                 | 9.433  | 9.266                    | 9.104                    | 8.951 | 8.801  | 8.659 | 8.519                   | 8.385 | 8.132 |
| 2-Amino-2-methylpropionic acid<br>(+ 1) | 2.419 <sup>1°C</sup>  |        | 2.380 <sup>12.5°C</sup>  |                          |       | 2.357  |       | 2.351 <sup>37.5°C</sup> |       | 2.356 |
| (0)                                     | 10.960 <sup>1°C</sup> |        | 10.580 <sup>12.5°C</sup> |                          |       | 10.205 |       | 9.872 <sup>37.5°C</sup> |       | 9.561 |
| 2-Aminopentanoic acid<br>(+ 1)          | 2.376 <sup>1°C</sup>  |        | 2.347                    |                          |       | 2.318  |       |                         | 2.309 | 2.313 |
| (0)                                     | 10.508 <sup>1°C</sup> |        |                          | 10.154 <sup>12.5°C</sup> |       | 9.808  |       | 9.490 <sup>37.5°C</sup> |       | 9.198 |
| 3-Aminopropionic acid<br>(+ 1)          | 3.656                 | 3.627  |                          | 3.583                    |       | 3.551  |       | 3.524                   | 3.517 |       |
| (0)                                     | 11.000                | 10.830 |                          | 10.526                   |       | 10.235 |       | 9.963                   | 9.842 |       |
| 4-Aminopyridine (+ 1)                   | 9.873                 | 9.704  | 9.549                    | 9.398                    | 9.252 | 9.114  | 8.978 | 8.846                   | 8.717 | 8.477 |
| Ammonium ion (+ 1)                      | 10.081                | 9.904  | 9.731                    | 9.564                    | 9.400 | 9.245  | 9.093 | 8.947                   | 8.805 | 8.539 |
| Arginine<br>(+ 1)                       | 1.914                 | 1.885  | 1.870                    | 1.849                    | 1.837 | 1.823  | 1.814 | 1.801                   | 1.800 | 1.787 |
| (0)                                     | 9.718                 | 9.563  | 9.407                    | 9.270                    | 9.123 | 8.994  | 8.859 | 8.739                   | 8.614 | 8.385 |
| Barbituric acid<br>(+ 1)                |                       |        |                          | 3.969                    | 3.980 | 4.02   | 4.00  | 4.008                   | 4.017 | 4.032 |
| (0)                                     |                       |        |                          | 8.493                    | 8.435 | 8.372  | 8.302 | 8.227                   | 8.147 | 7.974 |
| Benzoic acid (0)                        |                       | 4.231  | 4.220                    | 4.215                    | 4.206 | 4.204  | 4.203 | 4.207                   | 4.219 | 4.223 |
| Boric acid (0)                          | 9.508                 | 9.439  | 9.380                    | 9.327                    | 9.280 | 9.236  | 9.197 | 9.161                   | 9.132 | 9.080 |
| Bromoacetic acid (0)                    |                       |        |                          | 2.875                    | 2.887 | 2.902  | 2.918 | 2.936                   |       |       |
| 3-Bromobenzoic acid (0)                 |                       |        |                          | 3.818                    | 3.813 | 3.810  | 3.808 | 3.810                   | 3.813 |       |
| 4-Bromobenzoic acid (0)                 |                       |        |                          | 4.011                    | 4.005 | 3.99   | 4.001 | 4.001                   | 4.003 |       |
| Bromopropynoic acid (0)                 |                       |        | 1.786                    | 1.814                    | 1.839 | 1.855  | 1.879 | 1.900                   | 1.919 |       |

|                                              |        |        |        |        |        |        |        |        |        |        |
|----------------------------------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 3- <i>tert</i> -Butylbenzoic acid (0)        |        |        |        | 4.266  | 4.231  | 4.199  | 4.170  | 4.143  | 4.119  |        |
| 4- <i>tert</i> -Butylbenzoic acid (0)        |        |        |        | 4.463  | 4.425  | 4.389  | 4.354  | 4.320  | 4.287  |        |
| 2-Butynoic acid (0)                          |        |        | 2.618  | 2.626  | 2.611  | 2.620  | 2.618  | 2.621  | 2.631  |        |
| Butyric acid (0)                             | 4.806  | 4.804  | 4.803  | 4.805  | 4.810  | 4.817  | 4.827  | 4.840  | 4.854  | 4.885  |
| <b>DL</b> - <i>N</i> -Carbamoylalanine (+ 1) |        | 3.898  | 3.894  | 3.891  | 3.890  | 3.892  | 3.896  | 3.902  | 3.908  | 3.931  |
| <i>N</i> -Carbamoylglycine (+ 1)             |        | 3.911  | 3.900  | 3.889  | 3.879  | 3.876  | 3.874  | 3.873  | 3.875  | 3.888  |
| Carbon dioxide + water                       |        |        |        |        |        |        |        |        |        |        |
| (0)                                          | 6.577  | 6.517  | 6.465  | 6.429  | 6.382  | 6.352  | 6.327  | 6.309  | 6.296  | 6.285  |
| (− 1)                                        | 10.627 | 10.558 | 10.499 | 10.431 | 10.377 | 10.329 | 10.290 | 10.250 | 10.220 | 10.172 |
| Chloroacetic acid (0)                        |        |        |        | 2.845  | 2.856  | 2.867  | 2.883  | 2.900  |        |        |
| 3-Chlorobenzoic acid (0)                     |        |        |        | 3.838  | 3.831  | 3.83   | 3.825  | 3.826  | 3.829  |        |
| 4-Chlorobenzoic acid (0)                     |        |        |        | 4.000  | 3.991  | 3.986  | 3.981  | 3.980  | 3.981  |        |
| Chloropropynoic acid (0)                     |        |        | 1.766  | 1.796  | 1.820  | 1.845  | 1.864  | 1.879  | 1.893  |        |
| Citric acid                                  |        |        |        |        |        |        |        |        |        |        |
| (0)                                          | 3.220  | 3.200  | 3.176  | 3.160  | 3.142  | 3.128  | 3.116  | 3.109  | 3.099  | 3.095  |
| (− 1)                                        | 4.837  | 4.813  | 4.797  | 4.782  | 4.769  | 4.761  | 4.755  | 4.751  | 4.750  | 4.757  |
| (− 2)                                        | 6.393  | 6.386  | 6.383  | 6.384  | 6.388  | 6.396  | 6.406  | 6.423  | 6.439  | 6.484  |
| Cyanoacetic acid (0)                         |        | 2.445  | 2.447  | 2.452  | 2.460  | 2.460  | 2.482  | 2.496  | 2.511  |        |
| 2-Cyano-2-methylpropionic acid               |        |        |        |        |        |        |        |        |        |        |
| (0)                                          |        | 2.342  | 2.360  | 2.379  | 2.400  | 2.422  | 2.446  | 2.471  | 2.498  |        |
| 5,5-Diethylbarbituric acid (0)               | 8.40   | 8.30   | 8.22   | 8.169  | 8.094  | 8.020  | 7.948  | 7.877  | 7.808  | 7.673  |
| Diethylmalonic acid                          |        |        |        |        |        |        |        |        |        |        |
| (0)                                          |        |        | 2.129  | 2.136  | 2.144  | 2.151  | 2.160  | 2.172  | 2.187  |        |
| (− 1)                                        |        |        | 7.400  | 7.401  | 7.408  | 7.417  | 7.428  | 7.441  | 7.457  |        |
| 2,3-Dimethylbenzoic acid (0)                 |        |        |        | 3.663  | 3.687  | 3.771  | 3.726  | 3.762  | 3.788  |        |
| 2,4-Dimethylbenzoic acid (0)                 |        |        |        | 4.154  | 4.187  | 4.217  | 4.244  | 4.268  | 4.290  |        |
| 2,5-Dimethylbenzoic acid (0)                 |        |        |        | 3.911  | 3.954  | 3.990  | 4.020  | 4.045  | 4.065  |        |
| 2,6-Dimethylbenzoic acid (0)                 |        |        |        | 3.234  | 3.304  | 3.362  | 3.409  | 3.445  | 3.472  |        |
| 3,5-Dimethylbenzoic acid (0)                 |        |        |        | 4.292  | 4.299  | 4.302  | 4.304  | 4.306  | 4.306  |        |
| <i>N,N'</i> -Dimethylethyleneamine-          |        |        |        |        |        |        |        |        |        |        |
| <i>N,N'</i> -diacetic acid                   |        |        |        |        |        |        |        |        |        |        |
| (0)                                          | 6.294  |        | 6.169  |        | 6.047  |        | 5.926  |        | 5.803  |        |
| (− 1)                                        | 10.446 |        | 10.268 |        | 10.068 |        | 9.882  |        | 9.684  |        |
| <i>N,N</i> -Dimethylglycine (0)              |        | 10.34  |        | 10.14  |        | 9.94   |        | 9.76   |        |        |
| 3,5-Dinitrobenzoic acid (0)                  |        |        | 2.60   |        | 2.73   |        | 2.85   |        | 2.96   | 3.07   |

**TABLE 8.9** Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*Continued*)

| Substance                           | Temperature, °C |       |                         |        |       |       |       |                         |       |       |
|-------------------------------------|-----------------|-------|-------------------------|--------|-------|-------|-------|-------------------------|-------|-------|
|                                     | 0               | 5     | 10                      | 15     | 20    | 25    | 30    | 35                      | 40    | 50    |
| 2-Ethylbutyric acid (0)             | 4.623           |       | 4.664                   |        | 4.710 | 4.751 | 4.758 |                         | 4.812 | 4.869 |
| 5-Ethyl-5-phenylbarbituric acid (0) |                 |       |                         | 7.592  | 7.517 | 7.445 | 7.377 | 7.311                   | 7.248 | 7.130 |
| Fluoroacetic acid (0)               |                 |       |                         | 2.555  | 2.571 | 2.586 | 2.604 | 2.624                   |       |       |
| Formic acid (0)                     | 3.786           | 3.772 | 3.762                   | 3.757  | 3.753 | 3.751 | 3.752 | 3.758                   | 3.766 | 3.782 |
| 2-Furancarboxylic acid (0)          |                 |       |                         |        |       | 3.164 | 3.200 | 3.216                   | 3.239 |       |
| Glucose-1-phosphate (0)             |                 | 6.506 | 6.500                   | 6.499  | 6.500 | 6.504 | 6.510 | 6.519                   | 6.531 | 6.561 |
| Glycerol-1-phosphoric acid (− 1)    |                 | 6.642 | 6.641                   | 6.643  | 6.648 | 6.656 | 6.666 | 6.679                   | 6.695 | 6.733 |
| Glycerol-2-phosphoric acid (0)      |                 | 1.223 | 1.245                   | 1.271  | 1.301 | 1.335 | 1.372 | 1.413                   | 1.457 | 1.554 |
| (− 1)                               |                 | 6.657 | 6.650                   | 6.646  | 6.646 | 6.650 | 6.657 | 6.666                   | 6.679 | 6.712 |
| Glycine (+ 1)                       |                 |       | 2.397                   | 2.380  | 2.36  | 2.351 | 2.34  | 2.33                    | 2.327 | 2.32  |
| (0)                                 |                 | 10.34 | 10.193                  | 10.044 | 9.91  | 9.780 | 9.65  | 9.53                    | 9.412 | 9.19  |
| Glycolic acid (0)                   | 3.875           |       | 3.844 <sup>12.5°C</sup> |        |       | 3.831 |       | 3.833 <sup>37.5°C</sup> |       | 3.849 |
| Glycylasparagine (+ 1)              |                 | 2.968 | 2.958                   | 2.952  | 2.943 | 2.942 | 2.942 | 2.944                   | 2.947 | 2.959 |
| N-Glycylglycine (+ 1)               | 3.201           |       |                         |        |       | 3.126 |       |                         |       | 3.159 |
|                                     |                 |       | 8.594 <sup>12.5°C</sup> |        |       | 8.252 |       | 7.948 <sup>37.5°C</sup> |       | 7.668 |
| Hexanoic acid (0)                   | 4.840           |       | 4.839                   |        | 4.849 |       | 4.865 |                         | 4.890 | 4.920 |
| Hydrogen cyanide (0)                |                 |       | 9.63                    | 9.49   | 9.36  | 9.21  | 9.11  | 8.99                    | 8.88  |       |
| Hydrogen peroxide (0)               | 12.23           |       |                         | 11.86  | 11.75 | 11.65 | 11.55 | 11.45                   |       | 11.21 |
| Hydrogen sulfide (0)                |                 | 7.33  | 7.24                    | 7.13   | 7.05  | 6.97  | 6.90  | 6.82                    | 6.79  | 6.69  |
| (− 1)                               |                 | 13.5  |                         | 13.2   |       | 12.90 | 12.75 | 12.6                    |       |       |
| 4-Hydroxybenzoic acid (0)           |                 |       |                         | 4.596  | 4.586 | 4.582 | 4.577 | 4.576                   | 4.578 |       |
| Hydroxylamine (0)                   |                 |       |                         | 6.186  | 6.063 | 5.948 |       | 5.730                   |       |       |
| 2-Hydroxy-1-naphthoic acid (0)      |                 |       |                         |        | 3.29  |       | 3.24  |                         | 3.19  | 3.26  |
| (− 1)                               |                 |       |                         |        | 9.68  |       | 9.65  |                         | 9.61  | 9.58  |

|                                           |                                               |                |                                                     |                |                 |                |                |                                                    |                      |                |
|-------------------------------------------|-----------------------------------------------|----------------|-----------------------------------------------------|----------------|-----------------|----------------|----------------|----------------------------------------------------|----------------------|----------------|
| 4-Hydroxyproline<br>(+ 1)<br>(0)          | 1.900 <sup>1°C</sup><br>10.274 <sup>1°C</sup> |                | 1.850 <sup>12.5°C</sup><br>9.958 <sup>12.5°C</sup>  |                |                 | 1.818<br>9.662 |                | 1.798 <sup>37.5°C</sup><br>9.394 <sup>37.5°C</sup> |                      | 1.796<br>9.138 |
| 2-Hydroxypropionic acid (0)               | 3.880                                         | 3.873          | 3.868                                               | 3.861          | 3.857           | 3.858          | 3.861          | 3.867                                              | 3.873                | 3.895          |
| DL-2-Hydroxysuccinic acid<br>(0)<br>(− 1) | 3.537<br>5.119                                | 3.520<br>5.108 | 3.494<br>5.098                                      | 3.482<br>5.096 | 3.472<br>5.096  | 3.458<br>5.097 | 3.452<br>5.099 | 3.446<br>5.104                                     | 3.444<br>5.117       | 3.445<br>5.149 |
| Hypobromous acid (0)                      |                                               |                |                                                     | 8.83           |                 | 8.60           |                | 8.47                                               | 8.37 <sup>45°C</sup> |                |
| Hypochlorous acid (0)                     | 7.82                                          | 7.75           | 7.69                                                | 7.63           | 7.58            | 7.54           | 7.50           | 7.46                                               |                      | 7.05           |
| Imidazole (+ 1)                           | 7.581                                         | 7.467          | 7.334                                               | 7.216          | 7.103           | 6.993          | 6.887          | 6.784                                              | 6.685                | 6.497          |
| Iodoacetic acid (0)                       |                                               |                |                                                     | 3.143          | 3.158           | 3.175          | 3.193          | 3.213                                              |                      |                |
| DL-Isoleucine<br>(+ 1)<br>(0)             | 2.365<br>10.460                               |                | 2.338 <sup>12.5°C</sup><br>10.100 <sup>12.5°C</sup> |                |                 | 2.318<br>9.758 |                | 2.317 <sup>37.5°C</sup><br>9.439 <sup>37.5°C</sup> |                      | 2.332<br>9.157 |
| Isopropylmalonic acid,<br>mononitrile (0) |                                               | 2.299          | 2.320                                               | 2.343          | 2.365           | 2.401          | 2.427          | 2.452                                              | 2.481                |                |
| Lactic acid (0)                           | 3.880                                         | 3.873          | 3.868                                               | 3.862          | 3.857           | 3.858          | 3.861          | 3.867                                              | 3.873                | 3.895          |
| Lead sulfate, pK <sub>sp</sub>            | 8.01                                          |                |                                                     | 7.87           |                 | 7.80           |                | 7.73                                               |                      | 7.63           |
| DL-Leucine<br>(+ 1)<br>(0)                | 2.383 <sup>1°C</sup><br>10.458 <sup>1°C</sup> |                | 2.348 <sup>12.5°C</sup><br>10.095 <sup>1.5°C</sup>  |                |                 | 2.328<br>9.744 |                | 2.327 <sup>37.5°C</sup><br>9.434 <sup>37.5°C</sup> |                      | 2.333<br>9.142 |
| Malonic acid (− 1)                        | 5.670                                         | 5.665          | 5.667                                               | 5.673          | 5.683           | 5.696          | 5.710          | 5.730                                              | 5.753                | 5.803          |
| Mannose (0)                               |                                               |                | 12.45                                               |                |                 | 12.08          |                |                                                    | 11.81                |                |
| Mercury(I) chloride, pK <sub>sp</sub>     |                                               |                | 18.65                                               | 18.48          | 18.27           | 17.88          |                | 16.79                                              |                      |                |
| Methanol (solvent), pK <sub>auto</sub>    |                                               | 17.12          |                                                     | 16.84          |                 | 16.71          | 16.65          | 16.53                                              |                      |                |
| Methylamine (+ 1)                         | 11.496                                        |                | 11.130                                              |                | 10.787          | 10.62          | 10.466         |                                                    | 10.161               | 9.876          |
| Methylaminodiacetic acid<br>(0)<br>(− 1)  | 2.138<br>10.474                               |                | 2.142<br>10.287                                     |                | 2.146<br>10.088 |                | 2.150<br>9.920 |                                                    | 2.154<br>9.763       |                |
| 3-Methylbenzoic acid (0)                  |                                               |                |                                                     | 4.303          | 4.285           | 4.269          | 4.256          | 4.244                                              | 4.235                |                |
| 4-Methylbenzoic acid (0)                  |                                               |                |                                                     | 4.390          | 4.376           | 4.362          | 4.349          | 4.336                                              | 4.322                |                |
| 3-Methylbutyric acid (0)                  | 4.726                                         |                | 4.742                                               |                | 4.767           |                | 4.794          |                                                    | 4.831                | 4.871          |
| 4-Methylpentanoic acid (0)                | 4.827                                         |                | 4.827                                               |                | 4.837           |                | 4.853          |                                                    | 4.879                | 4.908          |

**TABLE 8.9** Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*Continued*)

| Substance                            | Temperature, °C |        |                          |        |        |        |        |                          |        |        |
|--------------------------------------|-----------------|--------|--------------------------|--------|--------|--------|--------|--------------------------|--------|--------|
|                                      | 0               | 5      | 10                       | 15     | 20     | 25     | 30     | 35                       | 40     | 50     |
| 5-Methyl-5-phenylbarbituric acid (0) |                 |        |                          | 8.104  | 8.057  | 8.011  | 7.966  | 7.922                    | 7.879  | 7.797  |
| 2-Methylpropionic acid (0)           | 4.825           |        | 4.827                    |        | 4.840  | 4.853  | 4.886  |                          | 4.918  | 4.955  |
| 2-Methyl-2-propylamine (+ 1)         |                 | 11.439 | 11.240                   | 11.048 | 10.862 | 10.682 | 10.511 | 10.341                   |        |        |
| Nitric acid (0)                      | − 1.65          |        |                          |        |        | − 1.38 |        |                          |        | − 1.20 |
| Nitrilotriacetic acid (0)            | 1.69            |        | 1.65                     |        | 1.65   |        | 1.66   |                          | 1.67   |        |
| (− 1)                                | 2.95            |        | 2.95                     |        | 2.94   |        | 2.96   |                          | 2.98   |        |
| (− 2)                                | 10.59           |        | 10.45                    |        | 10.33  |        | 10.23  |                          |        |        |
| 4-Nitrobenzoic acid (0)              |                 |        |                          | 3.448  | 3.444  | 3.441  | 3.441  | 3.442                    | 3.445  |        |
| Nitrous acid (0)                     |                 |        |                          | 3.244  | 3.177  | 3.138  |        | 3.100                    |        |        |
| DL-Norleucine (+ 1)                  | 2.394           |        | 2.356 <sup>12.5°C</sup>  |        |        | 2.335  |        | 2.324 <sup>37.5°C</sup>  |        | 2.328  |
| (0)                                  | 10.564          |        | 10.190 <sup>12.5°C</sup> |        |        | 9.834  |        | 9.513 <sup>37.5°C</sup>  |        | 9.224  |
| Oxalic acid (− 1)                    | 4.210           | 4.216  | 4.227                    | 4.240  | 4.254  | 4.272  | 4.295  | 4.318                    | 4.349  | 4.409  |
| 2,4-Pentanedione (0)                 | 9.07            |        |                          |        |        | 8.95   |        |                          | 8.90   |        |
| Pentanoic acid (0)                   | 4.823           |        | 4.763                    |        | 4.835  | 4.842  | 4.851  |                          | 4.861  | 4.906  |
| Phenylalanine (0)                    |                 |        | 9.75                     |        |        | 9.31   |        |                          | 8.96   |        |
| Phosphoric acid (0)                  | 2.056           | 2.073  | 2.088                    | 2.107  | 2.127  | 2.148  | 2.171  | 2.196                    | 2.224  | 2.277  |
| (− 1)                                | 7.313           | 7.282  | 7.254                    | 7.231  | 7.213  | 7.198  | 7.189  | 7.185                    | 7.181  | 7.183  |
| o-Phthalic acid (0)                  | 2.925           | 2.927  | 2.931                    | 2.937  | 2.943  | 2.950  | 2.958  | 2.967                    | 2.978  | 3.001  |
| (− 1)                                | 5.432           | 5.418  | 5.410                    | 5.405  | 5.405  | 5.408  | 5.416  | 5.427                    | 5.442  | 5.485  |
| Piperidine (+ 1)                     | 11.963          | 11.786 | 11.613                   | 11.443 | 11.280 | 11.123 | 10.974 | 10.818                   | 10.670 | 10.384 |
| Proline (+ 1)                        | 2.011           |        | 1.964 <sup>12.5°C</sup>  |        |        | 1.952  |        | 1.950 <sup>37.5°C</sup>  |        | 1.958  |
| (0)                                  | 11.296          |        | 10.972 <sup>12.5°C</sup> |        |        | 10.640 |        | 10.342 <sup>37.5°C</sup> |        | 10.064 |
| Propenoic acid (0)                   |                 |        |                          | 4.267  | 4.250  | 4.247  | 4.249  | 4.267                    | 4.301  |        |

|                                   |                      |                        |                          |        |        |       |       |                         |       |       |
|-----------------------------------|----------------------|------------------------|--------------------------|--------|--------|-------|-------|-------------------------|-------|-------|
| N-Propionylglycine (+ 1)          |                      | 3.728                  | 3.723                    | 3.718  | 3.716  | 3.718 | 3.721 | 3.725                   | 3.731 | 3.750 |
| Propynoic acid (0)                |                      |                        | 1.791                    | 1.829  | 1.867  | 1.887 | 1.940 | 1.932                   | 1.963 |       |
| Pyrrolidine (+ 1)                 | 12.17                | 11.98                  | 11.81                    | 11.63  | 11.43  | 11.30 | 11.15 | 10.99                   | 10.84 | 11.56 |
| Serine                            |                      |                        |                          |        |        |       |       |                         |       |       |
| (+ 1)                             | 2.296 <sup>1°C</sup> |                        | 2.232 <sup>12.5°C</sup>  |        |        | 2.186 |       | 2.154 <sup>37.5°C</sup> |       | 2.132 |
| (0)                               | 9.880 <sup>1°C</sup> |                        | 9.542 <sup>12.5°C</sup>  |        |        | 9.208 |       | 8.904 <sup>37.5°C</sup> |       | 8.628 |
| Silver bromide, pK <sub>sp</sub>  |                      | 13.33                  |                          | 12.83  | 12.57  | 12.30 | 12.07 | 11.83                   | 11.61 | 11.19 |
| Silver chloride, pK <sub>sp</sub> |                      | 10.595                 |                          | 10.152 |        | 9.749 |       | 9.381                   | 9.21  | 8.88  |
| Succinic acid                     |                      |                        |                          |        |        |       |       |                         |       |       |
| (0)                               | 4.285                | 4.263                  | 4.245                    | 4.232  | 4.218  | 4.207 | 4.198 | 4.191                   | 4.188 | 4.186 |
| (− 1)                             | 5.674                | 5.660                  | 5.649                    | 5.642  | 5.639  | 5.635 | 6.541 | 5.647                   | 5.654 | 5.680 |
| Sulfuric acid (− 1)               | 1.778                | 1.812 <sup>4.3°C</sup> |                          | 1.894  |        | 1.987 | 2.05  | 2.095                   | 2.17  | 2.246 |
| Sulfurous acid (0)                | 1.63                 |                        | 1.74                     |        |        | 1.89  |       | 1.98                    |       | 2.12  |
| D-Tartaric acid                   |                      |                        |                          |        |        |       |       |                         |       |       |
| (0)                               | 3.118                | 3.095                  | 3.075                    | 3.057  | 3.044  | 3.036 | 3.025 | 3.019                   | 3.018 | 3.021 |
| (− 1)                             | 4.426                | 4.407                  | 4.391                    | 4.381  | 4.372  | 4.366 | 4.365 | 4.367                   | 4.372 | 4.391 |
| 2,3,5,6-Tetramethylbenzoic acid   |                      |                        |                          | 3.310  | 3.367  | 3.415 | 3.453 | 3.483                   | 3.505 |       |
| (0)                               |                      |                        |                          |        |        |       |       |                         |       |       |
| Threonine                         |                      |                        |                          |        |        |       |       |                         |       |       |
| (+ 1)                             | 2.200 <sup>1°C</sup> |                        | 2.132 <sup>12.5°C</sup>  |        |        | 2.088 |       | 2.070 <sup>37.5°C</sup> |       | 2.055 |
| (0)                               | 9.748 <sup>1°C</sup> |                        | 9.420 <sup>12.5°C</sup>  |        |        | 9.100 |       | 8.812 <sup>37.5°C</sup> |       | 8.548 |
| o-Toluidine (0)                   |                      |                        |                          | 4.58   | 4.495  | 4.45  | 4.345 | 4.28                    | 4.20  |       |
| 1,2,4-Triazole                    |                      |                        |                          |        |        |       |       |                         |       |       |
| (+ 1)                             |                      |                        |                          | 2.451  | 2.418  | 2.386 | 2.327 |                         |       |       |
| (0)                               |                      |                        |                          | 10.205 | 10.083 | 9.972 | 9.768 |                         |       |       |
| 3,4,5-Trihydroxybenzoic acid (0)  |                      |                        |                          |        | 4.19   |       | 4.30  |                         | 4.38  | 4.53  |
| Tris(2-hydroxyethyl)amine (+ 1)   | 8.290                | 8.173                  | 8.067                    | 7.963  | 7.861  | 7.762 | 7.666 | 7.570                   | 7.477 | 7.299 |
| 2,4,6-Trimethylbenzoic acid (0)   |                      |                        |                          | 3.325  | 3.391  | 3.448 | 3.498 | 3.541                   | 3.577 |       |
| 3-Trimethylsilylbenzoic acid (0)  |                      |                        |                          | 4.142  | 4.116  | 4.089 | 4.060 | 4.029                   | 3.996 |       |
| 4-Trimethylsilylbenzoic acid (0)  |                      |                        |                          | 4.270  | 4.230  | 4.192 | 4.155 | 4.119                   | 4.084 |       |
| β-Ureidopropionic acid (0)        |                      | 4.514                  | 4.505                    | 4.497  | 4.490  | 4.487 | 4.486 | 4.486                   | 4.488 | 4.500 |
| DL-Valine                         |                      |                        |                          |        |        |       |       |                         |       |       |
| (+ 1)                             | 2.320                |                        | 2.297 <sup>12.5°C</sup>  |        |        | 2.296 |       | 2.292 <sup>37.5°C</sup> |       | 2.310 |
| (0)                               | 10.413               |                        | 10.064 <sup>12.5°C</sup> |        |        | 9.719 |       | 9.405 <sup>37.5°C</sup> |       | 9.124 |



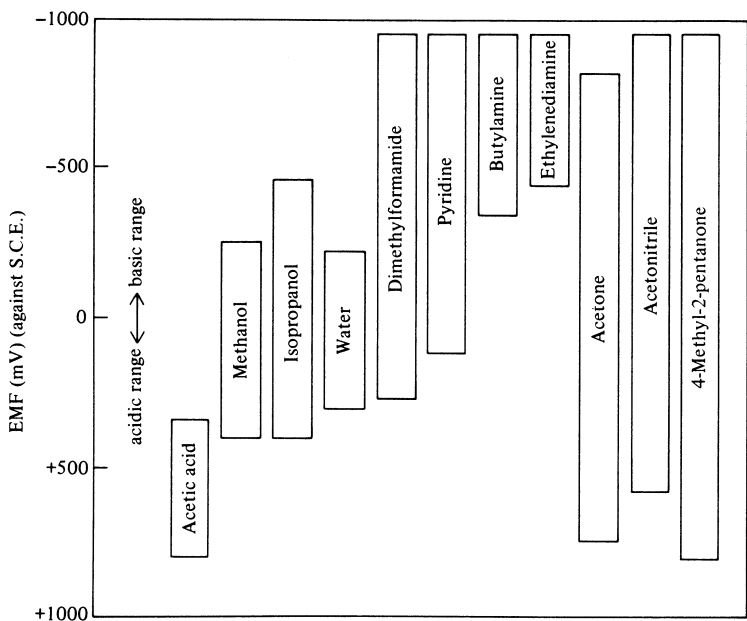


FIGURE 8.1 Approximate potential ranges in nonaqueous solvents.

TABLE 8.10 Properties of Common Acid-Base Solvents

| Solvent                                       | Potential Span, mV | − log K <sub>s</sub> | Dielectric Constant, 25°C |
|-----------------------------------------------|--------------------|----------------------|---------------------------|
| Acetic acid                                   | 400                | 14.5                 | 6.1(20°)                  |
| Acetic anhydride                              | 800                | 14.5                 | 20.7(20°)                 |
| Acetone                                       | 1600               |                      | 20.7                      |
| Acetonitrile                                  | 1600               | 26.5                 | 37.5(20°)                 |
| Ammonia (at − 50°C)                           |                    | 33                   | 22(− 33°)                 |
| n-Butanol                                     | 900                |                      | 17.1                      |
| n-Butylamine                                  | 500                |                      | 4.88(20°)                 |
| Chlorobenzene                                 | 1500               |                      | 5.62                      |
| N,N-Dimethylformamide                         | 1300               | 18.0                 | 36.71                     |
| Dimethylsulfoxide                             |                    | 17.3                 | 46.6                      |
| Ethanol                                       | 800                | 19.1                 | 24.55                     |
| Ethanolamine                                  |                    | 5.1                  | 37.7                      |
| Ethyl acetate                                 | 1500               |                      | 6.02                      |
| Ethylenediamine                               | 500                | 15.3                 | 14.2(20°)                 |
| Formic acid                                   | 200                | 6.2                  | 58.5                      |
| Methanol                                      | 800                | 16.7                 | 32.7                      |
| 4-Methyl-2-pentanone (methyl isobutyl ketone) | 1600               | 25.0                 | 13.1(20°)                 |
| Nitromethane                                  | 1000               |                      | 35.8(30°)                 |
| 2-Propanol                                    | 900                |                      | 19.92                     |
| Pyridine                                      | 1000               |                      | 12.3                      |
| Sulfuric acid                                 |                    | 3.85                 | 101                       |
| Water                                         | 800                | 14.0                 | 78.3                      |

**TABLE 8.11**  $pK_a$  Values for Proton-Transfer Reactions in Nonaqueous Solvents

| Acid                               | Methanol | Ethanol | Other Solvents                                   |
|------------------------------------|----------|---------|--------------------------------------------------|
| Acetic acid                        | 9.52     | 10.32   | 11.4 <sup>a</sup> , 9.75 <sup>d</sup>            |
| <i>p</i> -Aminobenzoic acid        | 10.25    |         |                                                  |
| Ammonium ion                       | 10.7     |         | 6.40 <sup>b</sup>                                |
| Anilinium ion                      | 6.0      | 5.70    |                                                  |
| Benzoic acid                       |          | 10.72   | 10.0 <sup>a</sup>                                |
| Bromocresol purple                 | 11.3     | 11.5    |                                                  |
| Bromocresol green                  | 9.8      | 10.65   |                                                  |
| Bromophenol blue                   | 8.9      | 9.5     |                                                  |
| Bromothymol blue                   | 12.4     | 13.2    |                                                  |
| Di- <i>n</i> -butylammonium ion    |          |         | 10.3 <sup>a</sup>                                |
| <i>o</i> -Chloroanilinium ion      | 3.4      |         |                                                  |
| Cyanoacetic acid                   |          | 7.49    |                                                  |
| 2,5-Dichloroanilinium ion          |          |         | 9.48 <sup>b</sup>                                |
| Dimethylaminoazobenzene            |          | 5.2     | 6.32 <sup>b</sup>                                |
| <i>N,N'</i> -Dimethylanilinium ion |          | 4.37    |                                                  |
| Formic acid                        |          | 9.15    |                                                  |
| Hydrobromic acid                   |          |         | 5.5 <sup>c</sup>                                 |
| Hydrochloric acid                  |          |         | 8.55 <sup>b</sup> , 8.9 <sup>c</sup>             |
| Methyl orange                      | 3.8      | 3.4     |                                                  |
| Methyl red (acid range)            | 4.1      | 3.55    |                                                  |
| (alkaline range)                   | 9.2      | 10.45   |                                                  |
| Methyl yellow                      | 3.4      | 3.55    |                                                  |
| Neutral red                        | 8.2      | 8.2     |                                                  |
| <i>o</i> -Nitrobenzoic acid        | 7.6      |         |                                                  |
| <i>m</i> -Nitrobenzoic acid        | 8.3      |         |                                                  |
| <i>p</i> -Nitrobenzoic acid        | 8.4      |         |                                                  |
| Perchloric acid                    |          |         | 4.87 <sup>b</sup>                                |
| Phenol                             | 14.0     |         |                                                  |
| Phenol red                         | 12.8     | 13.4    |                                                  |
| Phthalic acid, $pK_2$              | 11.65    |         | 11.5 <sup>d</sup> , 6.10 <sup>d</sup> ( $pK_1$ ) |
| Picric acid                        | 3.8      | 3.8     | 8.9 <sup>c</sup>                                 |
| Pyridinium ion                     |          |         | 6.1 <sup>b</sup>                                 |
| Salicylic acid                     | 8.7      | 7.9     |                                                  |
| Stearic acid                       | 10.0     |         |                                                  |
| Succinic acid, $pK_2$              | 11.4     |         |                                                  |
| Sulfuric acid, $pK_1$              |          |         | 7.24 <sup>b,c</sup>                              |
| Tartaric acid, $pK_2$              | 9.9      |         |                                                  |
| Thymol blue (alkaline range)       | 14.0     | 15.2    |                                                  |
| (acid range)                       | 4.7      | 5.35    |                                                  |
| Thymolbenzein (acid range)         | 3.5      |         |                                                  |
| (alkaline range)                   | 13.1     |         |                                                  |
| <i>p</i> -Toluenesulfonic acid     |          |         | 8.44 <sup>b</sup>                                |
| <i>p</i> -Toluidinium ion          |          | 6.24    |                                                  |
| Tribenzylammonium ion              |          |         | 5.40 <sup>b</sup>                                |
| Tropeoline 00                      | 2.2      |         |                                                  |
| Urea (protonated cation)           |          |         | 6.96 <sup>b</sup>                                |
| Veronal                            | 12.6     |         |                                                  |

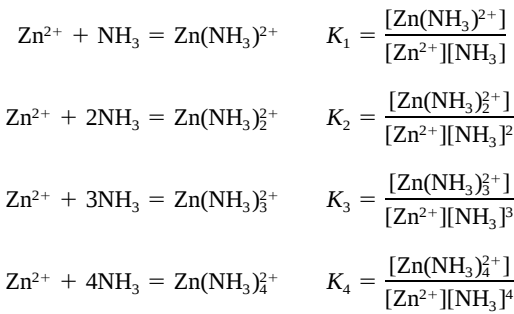
<sup>a</sup> Dimethylsulfoxide. <sup>b</sup> Glacial acetic acid. <sup>c</sup> Acetonitrile. <sup>d</sup> Acetone + 10% water.

8.2.2 Formation Constants of Metal Complexes

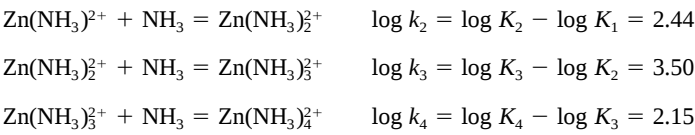
Each value listed in Tables 8.12 and 8.13 is the logarithm of the overall formation constant for the cumulative binding of a ligand  $L$  to the central metal cation  $M$ , viz.:

|                 | Cumulative<br>formation constant | Stepwise<br>stability constants |
|-----------------|----------------------------------|---------------------------------|
| $M + L = ML$    | $K_1$                            | $k_1$                           |
| $M + 2L = ML_2$ | $K_2$                            | $k_1 k_2$                       |
| .....           |                                  |                                 |
| $M + nL = ML_n$ | $K_n$                            | $k_1 k_2 \cdots k_n$            |

As an example, the entries in Table 8.12 for the zinc ammine complexes represent these equilibria:



If the stepwise stability or formation constants of the reactions are desired, for the first step  $\log K_1 = \log k_1 = 2.37$ . For the second and succeeding steps the equilibria and corresponding constants are as follows:



The reverse of the association or formation reactions would represent the dissociation or instability constant for the systems, i.e.,  $-\log K_f = \log K_{\text{instab}}$ .

The data in the tables generally refer to temperatures of about 20 to 25°C. Most of the values in Table 8.12 refer to zero ionic strength, but those in Table 8.13 often refer to a finite ionic strength.

**TABLE 8.12** Cumulative Formation Constants for Metal Complexes with Inorganic Ligands

|                 | $\log K_1$              | $\log K_2$ | $\log K_3$ | $\log K_4$ | $\log K_5$ | $\log K_6$ |
|-----------------|-------------------------|------------|------------|------------|------------|------------|
| <b>Ammonia</b>  |                         |            |            |            |            |            |
| Cadmium         | 2.65                    | 4.75       | 6.19       | 7.12       | 6.80       | 5.14       |
| Cobalt(II)      | 2.11                    | 3.74       | 4.79       | 5.55       | 5.73       | 5.11       |
| Cobalt(III)     | 6.7                     | 14.0       | 20.1       | 25.7       | 30.8       | 35.2       |
| Copper(I)       | 5.93                    | 10.86      |            |            |            |            |
| Copper(II)      | 4.31                    | 7.98       | 11.02      | 13.32      | 12.86      |            |
| Iron(II)        | 1.4                     | 2.2        |            |            |            |            |
| Manganese(II)   | 0.8                     | 1.3        |            |            |            |            |
| Mercury(II)     | 8.8                     | 17.5       | 18.5       | 19.28      |            |            |
| Nickel          | 2.80                    | 5.04       | 6.77       | 7.96       | 8.71       | 8.74       |
| Platinum(II)    |                         |            |            |            |            | 35.3       |
| Silver(I)       | 3.24                    | 7.05       |            |            |            |            |
| Zinc            | 2.37                    | 4.81       | 7.31       | 9.46       |            |            |
| <b>Bromide</b>  |                         |            |            |            |            |            |
| Astatine        | 2.51 [AtBr]             |            |            |            |            |            |
| Bismuth(III)    | 4.30                    | 5.55       | 5.89       | 7.82       |            | 9.70       |
| Bromine         | 1.24 [Br <sub>3</sub> ] |            |            |            |            |            |
| Cadmium         | 1.75                    | 2.34       | 3.32       | 3.70       |            |            |
| Cerium(III)     | 0.42                    |            |            |            |            |            |
| Copper(I)       |                         | 5.89       |            |            |            |            |
| Copper(II)      | 0.30                    |            |            |            |            |            |
| Gold(I)         |                         | 12.46      |            |            |            |            |
| Indium          | 1.30                    | 1.88       | 2.48       |            |            |            |
| Iodine          | 2.64 [IBr]              |            |            |            |            |            |
| Iron(III)       | -0.30                   | -0.50      |            |            |            |            |
| Lead            | 1.2                     | 1.9        |            | 1.1        |            |            |
| Mercury(II)     | 9.05                    | 17.32      | 19.74      | 21.00      |            |            |
| Palladium(II)   |                         |            |            | 13.1       |            |            |
| Platinum(II)    |                         |            |            | 20.5       |            |            |
| Rhodium(III)    |                         | 14.3       | 16.3       | 17.6       | 18.4       | 17.2       |
| Scandium        | 2.08                    | 3.08       |            |            |            |            |
| Silver(I)       | 4.38                    | 7.33       | 8.00       | 8.73       |            |            |
| Thallium(I)     | 0.93                    |            |            |            |            |            |
| Thallium(III)   | 9.7                     | 16.6       | 21.2       | 23.9       | 29.2       | 31.6       |
| Tin(II)         | 1.11                    | 1.81       | 1.46       |            |            |            |
| Uranium(IV)     | 0.18                    |            |            |            |            |            |
| Yttrium         | 1.32                    |            |            |            |            |            |
| <b>Chloride</b> |                         |            |            |            |            |            |
| Americium(III)  | 1.17                    |            |            |            |            |            |
| Antimony(III)   | 2.26                    | 3.49       | 4.18       | 4.72       |            |            |
| Bismuth(III)    | 2.44                    | 4.7        | 5.0        | 5.6        |            |            |
| Cadmium         | 1.95                    | 2.50       | 2.60       | 2.80       |            |            |
| Cerium(III)     | 0.48                    |            |            |            |            |            |
| Copper(I)       |                         | 5.5        | 5.7        |            |            |            |
| Copper(II)      | 0.1                     | -0.6       |            |            |            |            |
| Curium(III)     | 1.17                    |            |            |            |            |            |
| Gold(III)       |                         | 9.8        |            |            |            |            |
| Indium          | 1.42                    | 2.23       | 3.23       |            |            |            |
| Iron(II)        | 0.36                    |            |            |            |            |            |
| Iron(III)       | 1.48                    | 2.13       | 1.99       | 0.01       |            |            |
| Lead            | 1.62                    | 2.44       | 1.70       | 1.60       |            |            |
| Manganese(II)   | 0.96                    |            |            |            |            |            |
| Mercury(II)     | 6.74                    | 13.22      | 14.07      | 15.07      |            |            |

**TABLE 8.12** Cumulative Formation Constants for Metal Complexes with Inorganic Ligands (*Continued*)

|                                   | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$ | log $K_5$ | log $K_6$ |
|-----------------------------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Palladium(II)                     | 6.1       | 10.7      | 13.1      | 15.7      |           |           |
| Platinum(II)                      |           | 11.5      | 14.5      | 16.0      |           |           |
| Plutonium(III)                    | 1.17      |           |           |           |           |           |
| Silver(I)                         | 3.04      | 5.04      |           | 5.30      |           |           |
| Thallium(I)                       | 0.52      |           |           |           |           |           |
| Thallium(III)                     | 8.14      | 13.60     | 15.78     | 18.00     |           |           |
| Thorium                           | 1.38      | 0.38      |           |           |           |           |
| Tin(II)                           | 1.51      | 2.24      | 2.03      | 1.48      |           |           |
| Tin(IV)                           |           |           |           |           |           | 4         |
| Uranium(IV)                       | 0.8       |           |           |           |           |           |
| Uranium(VI)                       | 0.22      |           |           |           |           |           |
| Zinc                              | 0.43      | 0.61      | 0.53      | 0.20      |           |           |
| Zirconium                         | 0.9       | 1.3       | 1.5       | 1.2       |           |           |
| <b>Cyanide</b>                    |           |           |           |           |           |           |
| Cadmium                           | 5.48      | 10.60     | 15.23     | 18.78     |           |           |
| Copper(I)                         |           | 24.0      | 28.59     | 30.30     |           |           |
| Gold(I)                           |           | 38.3      |           |           |           |           |
| Iron(II)                          |           |           |           |           |           | 35        |
| Iron(III)                         |           |           |           |           |           | 42        |
| Mercury(II)                       |           |           |           | 41.4      |           |           |
| Nickel                            |           |           |           | 31.3      |           |           |
| Silver(I)                         |           | 21.1      | 21.7      | 20.6      |           |           |
| Zinc                              |           |           |           | 16.7      |           |           |
| <b>Fluoride</b>                   |           |           |           |           |           |           |
| Aluminum                          | 6.10      | 11.15     | 15.00     | 17.75     | 19.37     | 19.84     |
| Beryllium                         | 5.1       | 8.8       | 12.6      |           |           |           |
| Cerium(III)                       | 3.20      |           |           |           |           |           |
| Chromium(III)                     | 4.41      | 7.81      | 10.29     |           |           |           |
| Gadolinium                        | 3.46      |           |           |           |           |           |
| Gallium                           | 5.08      |           |           |           |           |           |
| Indium                            | 3.70      | 6.25      | 8.60      | 9.70      |           |           |
| Iron(III)                         | 5.28      | 9.30      | 12.06     |           |           |           |
| Lanthanum                         | 2.77      |           |           |           |           |           |
| Magnesium                         | 1.30      |           |           |           |           |           |
| Manganese(II)                     | 5.48      |           |           |           |           |           |
| Plutonium(III)                    | 6.77      |           |           |           |           |           |
| Scandium                          |           |           |           |           |           | 17.3      |
| Thallium(I)                       | 0.1       |           |           |           |           |           |
| Thallium(III) [TlO <sup>+</sup> ] | 6.44      |           |           |           |           |           |
| Thorium                           | 7.65      | 13.46     | 17.97     |           |           |           |
| Titanium(IV) [TiO <sup>2+</sup> ] | 5.4       | 9.8       | 13.7      | 18.0      |           |           |
| Uranium(VI)                       | 4.59      | 7.93      | 10.47     | 11.84     |           |           |
| Yttrium                           | 4.81      | 8.54      | 12.14     |           |           |           |
| Zirconium                         | 8.80      | 16.12     | 21.94     |           |           |           |
| <b>Hydroxide</b>                  |           |           |           |           |           |           |
| Aluminum                          | 9.27      |           |           | 33.03     |           |           |
| Antimony(III)                     |           | 24.3      | 36.7      | 38.3      |           |           |
| Arsenic [as AsO <sup>+</sup> ]    | 14.33     | 18.73     | 20.60     | 21.20     |           |           |
| Beryllium                         | 9.7       | 14.0      | 15.2      |           |           |           |
| Bismuth(III)                      | 12.7      | 15.8      |           | 35.2      |           |           |
| Cadmium                           | 4.17      | 8.33      | 9.02      | 8.62      |           |           |
| Cerium(III)                       | 14.6      |           |           |           |           |           |
| Cerium(IV)                        | 13.28     | 26.46     |           |           |           |           |

**TABLE 8.12** Cumulative Formation Constants for Metal Complexes with Inorganic Ligands (*Continued*)

|                                      | $\log K_1$ | $\log K_2$ | $\log K_3$                                      | $\log K_4$ | $\log K_5$ | $\log K_6$ |
|--------------------------------------|------------|------------|-------------------------------------------------|------------|------------|------------|
| Chromium(III)                        | 10.1       | 17.8       |                                                 | 29.9       |            |            |
| Copper(II)                           | 7.0        | 13.68      | 17.00                                           | 18.5       |            |            |
| Dysprosium                           | 5.2        |            |                                                 |            |            |            |
| Erbium(III)                          | 5.4        |            |                                                 |            |            |            |
| Gadolinium                           | 4.6        |            |                                                 |            |            |            |
| Gallium                              | 11.0       | 21.7       |                                                 | 34.3       | 38.0       | 40.3       |
| Indium                               | 9.9        | 19.8       |                                                 | 28.7       |            |            |
| Iodine                               | 9.49       | 11.24      |                                                 |            |            |            |
| Iron(II)                             | 5.56       | 9.77       | 9.67                                            | 8.58       |            |            |
| Iron(III)                            | 11.87      | 21.17      | 29.67                                           |            |            |            |
| Lanthanum                            | 3.3        |            |                                                 |            |            |            |
| Lead(II)                             | 7.82       | 10.85      | 14.58                                           |            |            | 61.0       |
| Lutetium                             | 6.6        |            |                                                 |            |            |            |
| Magnesium                            | 2.58       |            |                                                 |            |            |            |
| Manganese(II)                        | 3.90       |            | 8.3                                             |            |            |            |
| Neodymium                            | 5.5        |            |                                                 |            |            |            |
| Nickel                               | 4.97       | 8.55       | 11.33                                           |            |            |            |
| Praseodymium                         | 4.30       |            |                                                 |            |            |            |
| Plutonium(III)                       | 7.0        |            |                                                 |            |            |            |
| Plutonium(IV)                        | 12.39      |            |                                                 |            |            |            |
| Plutonium [as $\text{PuO}_2^{2+}$ ]  | 8.3        | 16.6       | 20.9                                            |            |            |            |
| Samarium(III)                        | 4.8        |            |                                                 |            |            |            |
| Scandium                             | 8.9        |            |                                                 |            |            |            |
| Tellurium(IV)                        |            |            | 41.6                                            | 53.0       | 64.8       | 72.0       |
| Thallium(III)                        | 12.86      | 25.37      |                                                 |            |            |            |
| Titanium(III)                        | 12.71      |            |                                                 |            |            |            |
| Uranium(IV)                          | 13.3       |            |                                                 |            | 41.2       |            |
| Uranium(VI) [as $\text{UO}_2^{2+}$ ] | 9.5        | 22.80      |                                                 | 32.4       |            |            |
| Vanadium(III)                        | 11.1       | 21.6       |                                                 |            |            |            |
| Vanadium(IV) [as $\text{VO}^{2+}$ ]  | 8.6        |            | [25.8 for $\text{V}_2\text{O}_4(\text{OH})^-$ ] |            |            |            |
| Vanadium(V) [as $\text{VO}^{3+}$ ]   |            | 25.2       |                                                 | 46.2       | 58.5       |            |
| Yttrium                              | 5.0        |            |                                                 |            |            |            |
| Zinc                                 | 4.40       | 11.30      | 14.14                                           | 17.66      |            |            |
| Zirconium                            | 14.3       | 28.3       | 41.9                                            | 55.3       |            |            |
| <b>Iodide</b>                        |            |            |                                                 |            |            |            |
| Bismuth                              | 3.63       |            |                                                 | 14.95      | 16.80      | 18.80      |
| Cadmium                              | 2.10       | 3.43       | 4.49                                            | 5.41       |            |            |
| Copper(I)                            |            | 8.85       |                                                 |            |            |            |
| Indium                               | 1.00       | 2.26       |                                                 |            |            |            |
| Iodine                               | 2.89       | 5.79       |                                                 |            |            |            |
| Iron(III)                            | 1.88       |            |                                                 |            |            |            |
| Lead                                 | 2.00       | 3.15       | 3.92                                            | 4.47       |            |            |
| Mercury(II)                          | 12.87      | 23.82      | 27.60                                           | 29.83      |            |            |
| Silver                               | 6.58       | 11.74      | 13.68                                           |            |            |            |
| Thallium(I)                          | 0.72       | 0.90       | 1.08                                            |            |            |            |
| Thallium(III)                        | 11.41      | 20.88      | 27.60                                           | 31.82      |            |            |
| <b>Iodate</b>                        |            |            |                                                 |            |            |            |
| Barium                               | 1.05       |            |                                                 |            |            |            |
| Calcium                              | 0.89       |            |                                                 |            |            |            |
| Magnesium                            | 0.72       |            |                                                 |            |            |            |
| Strontium                            | 1.00       |            |                                                 |            |            |            |
| Thorium                              | 2.88       | 4.79       | 7.15                                            |            |            |            |

**TABLE 8.12** Cumulative Formation Constants for Metal Complexes with Inorganic Ligands (*Continued*)

|                                   | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$ | log $K_5$ | log $K_6$ |
|-----------------------------------|-----------|-----------|-----------|-----------|-----------|-----------|
| <b>Nitrate</b>                    |           |           |           |           |           |           |
| Barium                            | 0.92      |           |           |           |           |           |
| Beryllium                         | 1.62      |           |           |           |           |           |
| Bismuth(III)                      | 1.26      |           |           |           |           |           |
| Cadmium                           | 0.40      |           |           |           |           |           |
| Calcium                           | 0.28      |           |           |           |           |           |
| Cerium(III)                       | 1.04      | 2.55      |           |           |           |           |
| Curium(III)                       | 0.57      |           |           |           |           |           |
| Hafnium                           | 0.92      | 2.43      | 4.32      | 6.40      | 8.48      | 10.29     |
| Iron(III)                         | 1.0       |           |           |           |           |           |
| Lanthanum                         | 0.26      | 0.69      | 1.27      |           |           |           |
| Lead                              | 1.18      |           |           |           |           |           |
| Mercury(II)                       | 0.35      |           |           |           |           |           |
| Neodymium                         | 0.52      | 1.18      |           |           |           |           |
| Neptunium(IV)                     | 0.38      |           |           |           |           |           |
| Plutonium(III)                    | 0.77      | 1.93      | 3.09      |           |           |           |
| Plutonium(IV)                     | 0.54      |           |           |           |           |           |
| Strontium                         | 0.82      |           |           |           |           |           |
| Thallium(I)                       | 0.33      |           |           |           |           |           |
| Thallium(III)                     | 0.92      |           |           |           |           |           |
| Thorium                           | 0.78      | 1.89      | 2.89      | 3.63      |           |           |
| Uranium(IV)                       | 0.20      | 0.37      |           |           |           |           |
| Uranium(VI)                       | 0.34      | 0.45      |           |           |           |           |
| Ytterbium                         | 0.45      | 1.30      | 2.42      |           |           |           |
| Zirconium [as $\text{ZrO}^{2+}$ ] |           | 1.91      |           | 3.54      |           |           |
| <b>Pyrophosphate</b>              |           |           |           |           |           |           |
| Barium                            | 4.6       |           |           |           |           |           |
| Calcium                           | 4.6       |           |           |           |           |           |
| Cadmium                           | 5.6       |           |           |           |           |           |
| Copper(II)                        | 6.7       | 9.0       |           |           |           |           |
| Lead                              |           | 5.3       |           |           |           |           |
| Magnesium                         | 5.7       |           |           |           |           |           |
| Nickel                            | 5.8       | 7.4       |           |           |           |           |
| Strontium                         | 4.7       |           |           |           |           |           |
| Yttrium                           |           | 9.7       |           |           |           |           |
| Zirconium                         |           | 6.5       |           |           |           |           |
| <b>Sulfate</b>                    |           |           |           |           |           |           |
| Cerium(III)                       | 3.40      |           |           |           |           |           |
| Erbium                            | 3.58      |           |           |           |           |           |
| Gadolinium                        | 3.66      |           |           |           |           |           |
| Holmium                           | 3.58      |           |           |           |           |           |
| Indium                            | 1.78      | 1.88      | 2.36      |           |           |           |
| Iron(III)                         | 2.03      | 2.98      |           |           |           |           |
| Lanthanum                         | 3.64      |           |           |           |           |           |
| Neodymium                         | 3.64      |           |           |           |           |           |
| Nickel                            | 2.4       |           |           |           |           |           |
| Plutonium(IV)                     | 3.66      |           |           |           |           |           |
| Praseodymium                      | 3.62      |           |           |           |           |           |
| Samarium                          | 3.66      |           |           |           |           |           |
| Thorium                           | 3.32      | 5.50      |           |           |           |           |
| Uranium(IV)                       | 3.24      | 5.42      |           |           |           |           |
| Uranium(VI)                       | 1.70      | 2.45      | 3.30      |           |           |           |

**TABLE 8.12** Cumulative Formation Constants for Metal Complexes with Inorganic Ligands (*Continued*)

|                    | $\log K_1$ | $\log K_2$ | $\log K_3$ | $\log K_4$ | $\log K_5$ | $\log K_6$ |
|--------------------|------------|------------|------------|------------|------------|------------|
| Yttrium            | 3.47       |            |            |            |            |            |
| Ytterbium          | 3.58       |            |            |            |            |            |
| Zirconium          | 3.79       | 6.64       | 7.77       |            |            |            |
| <b>Sulfite</b>     |            |            |            |            |            |            |
| Copper(I)          | 7.5        | 8.5        | 9.2        |            |            |            |
| Mercury(II)        |            | 22.66      |            |            |            |            |
| Silver             | 5.30       | 7.35       |            |            |            |            |
| <b>Thiocyanate</b> |            |            |            |            |            |            |
| Bismuth            | 1.15       | 2.26       | 3.41       | 4.23       |            |            |
| Cadmium            | 1.39       | 1.98       | 2.58       | 3.6        |            |            |
| Chromium(III)      | 1.87       | 2.98       |            |            |            |            |
| Cobalt(II)         | -0.04      | -0.70      | 0          | 3.00       |            |            |
| Copper(I)          | 12.11      | 5.18       |            |            |            |            |
| Gold(I)            |            | 23         |            | 42         |            |            |
| Indium             | 2.58       | 3.00       | 4.63       |            |            |            |
| Iron(III)          | 2.95       | 3.36       |            |            |            |            |
| Mercury(II)        |            | 17.47      |            | 21.23      |            |            |
| Nickel             | 1.18       | 1.64       | 1.81       |            |            |            |
| Ruthenium(III)     | 1.78       |            |            |            |            |            |
| Silver             |            | 7.57       | 9.08       | 10.08      |            |            |
| Thallium(I)        | 0.80       |            |            |            |            |            |
| Uranium(IV)        | 1.49       | 2.11       |            |            |            |            |
| Uranium(VI)        | 0.76       | 0.74       | 1.18       |            |            |            |
| Vanadium(III)      | 2.0        |            |            |            |            |            |
| Vanadium(IV)       | 0.92       |            |            |            |            |            |
| Zinc               | 1.62       |            |            |            |            |            |
| <b>Thiosulfate</b> |            |            |            |            |            |            |
| Cadmium            | 3.92       | 6.44       |            |            |            |            |
| Copper(I)          | 10.27      | 12.22      | 13.84      |            |            |            |
| Iron(III)          | 2.10       |            |            |            |            |            |
| Lead               |            | 5.13       | 6.35       |            |            |            |
| Mercury(II)        |            | 29.44      | 31.90      | 33.24      |            |            |
| Silver             | 8.82       | 13.46      |            |            |            |            |



**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands

Temperature is 25°C and ionic strengths are approaching zero unless indicated otherwise: (a) At 20°C, (b) at 30°C, (c) 0.1 *M* uni-univalent salt, (d) 1.0 *M* uni-univalent salt, (e) 2.0 *M* uni-univalent salt present.

|                                 | log <i>K</i> <sub>1</sub> | log <i>K</i> <sub>2</sub> | log <i>K</i> <sub>3</sub> | log <i>K</i> <sub>4</sub> |
|---------------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| <b>Acetate</b>                  |                           |                           |                           |                           |
| Ag(I)                           | 0.73                      | 0.64                      |                           |                           |
| Ba(II)                          | 0.41                      |                           |                           |                           |
| Ca(II)                          | 0.6                       |                           |                           |                           |
| Cd(II)                          | 1.5                       | 2.3                       | 2.4                       |                           |
| Ce(III)                         | 1.68                      | 2.69                      | 3.13                      | 3.18                      |
| Co(II)                          | 1.5                       | 1.9                       |                           |                           |
| Cr(III)                         | 1.80                      | 4.72                      |                           |                           |
| Cu(II) <i>a</i>                 | 2.16                      | 3.20                      |                           |                           |
| Fe(II) <i>c</i>                 | 3.2                       | 6.1                       | 8.3                       |                           |
| Fe(III) <i>a,d</i>              | 3.2                       |                           |                           |                           |
| In(III)                         | 3.50                      | 5.95                      | 7.90                      | 9.08                      |
| Hg(II)                          |                           | 8.43                      |                           |                           |
| La(III) <i>a,e</i>              | 1.56                      | 2.48                      | 2.98                      | 2.95                      |
| Mg(II)                          | 0.8                       |                           |                           |                           |
| Mn(II)                          | 9.84                      | 2.06                      |                           |                           |
| Ni(II)                          | 1.12                      | 1.81                      |                           |                           |
| Pb(II)                          | 2.52                      | 4.0                       | 6.4                       | 8.5                       |
| Rare earths <i>a,e</i>          | 1.6–1.9                   | 2.8–3.0                   | 3.3–3.7                   |                           |
| Sr(II)                          | 0.44                      |                           |                           |                           |
| Tl(III)                         |                           |                           |                           | 15.4                      |
| UO <sub>2</sub> (II) <i>a,e</i> | 2.38                      | 4.36                      | 6.34                      |                           |
| Y(III) <i>a,e</i>               | 1.53                      | 2.65                      | 3.38                      |                           |
| Zn(II)                          | 1.5                       |                           |                           |                           |
| <b>Acetylacetone</b>            |                           |                           |                           |                           |
| Al(III) <i>b</i>                | 8.6                       | 15.5                      |                           |                           |
| Be(II)                          | 7.8                       | 14.5                      |                           |                           |
| Cd(II)                          | 3.84                      | 6.66                      |                           |                           |
| Ce(III)                         | 5.30                      | 9.27                      | 12.65                     |                           |
| Cr(II)                          | 5.9                       | 11.7                      |                           |                           |
| Co(II)                          | 5.40                      | 9.54                      |                           |                           |
| Cu(II)                          | 8.27                      | 16.34                     |                           |                           |
| Dy(III) <i>b</i>                | 6.03                      | 10.70                     | 14.04                     |                           |
| Er(III) <i>b</i>                | 5.99                      | 10.67                     | 14.09                     |                           |
| Eu(III) <i>b</i>                | 5.87                      | 10.35                     | 13.64                     |                           |
| Fe(II)                          | 5.07                      | 8.67                      |                           |                           |
| Fe(III)                         | 11.4                      | 22.1                      | 26.7                      |                           |
| Ga(III)                         | 9.5                       | 17.9                      | 23.6                      |                           |
| Gd(III) <i>b</i>                | 5.90                      | 10.38                     | 13.79                     |                           |
| Hf(IV)                          | 8.7                       | 15.4                      | 21.8                      | 28.1                      |
| Ho(III)                         | 6.05                      | 10.73                     | 14.13                     |                           |
| In(III)                         | 8.0                       | 15.1                      |                           |                           |
| La(III) <i>b</i>                | 5.1                       | 8.90                      | 11.90                     |                           |
| Lu(III) <i>b</i>                | 6.23                      | 11.00                     | 13.63                     |                           |
| Mg(II)                          | 3.65                      | 6.27                      |                           |                           |
| Mn(II)                          | 4.24                      | 7.35                      |                           |                           |
| Mn(III)                         |                           |                           | 3.86                      |                           |
| Nd(III)                         | 5.6                       | 9.9                       | 13.1                      |                           |
| Ni(II) <i>a</i>                 | 6.06                      | 10.77                     | 13.09                     |                           |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                     | $\log K_1$ | $\log K_2$ | $\log K_3$ | $\log K_4$ |
|-------------------------------------|------------|------------|------------|------------|
| Pd(II) <i>b</i>                     | 16.2       | 27.1       |            |            |
| Pr(III) <i>b</i>                    | 5.4        | 9.5        | 12.5       |            |
| Pu(IV) <i>c</i>                     | 10.5       | 19.7       | 28.1       | 34.1       |
| Sc(III) <i>b</i>                    | 8.0        | 15.2       |            |            |
| Sm(III) <i>b</i>                    | 5.9        | 10.4       |            |            |
| Tb(III) <i>b</i>                    | 6.02       | 10.63      | 14.04      |            |
| Th(IV)                              | 8.8        | 16.2       | 22.5       | 26.7       |
| Tm(IV) <i>b</i>                     | 6.09       | 10.85      | 14.33      |            |
| U(IV) <i>a,c</i>                    | 8.6        | 17.0       | 23.4       | 29.5       |
| UO <sub>2</sub> (II) <i>b</i>       | 7.74       | 14.19      |            |            |
| VO(II)                              | 8.68       | 15.79      |            |            |
| V(II)                               | 5.4        | 10.2       | 14.7       |            |
| Y(III) <i>b</i>                     | 6.4        | 11.1       | 13.9       |            |
| Yb(III) <i>b</i>                    | 6.18       | 11.04      | 13.64      |            |
| Zn(II) <i>b</i>                     | 4.98       | 8.81       |            |            |
| Zr(IV)                              | 8.4        | 16.0       | 23.2       | 30.1       |
| <b>Alizarin red</b>                 |            |            |            |            |
| Cr(VI)                              | 4.7        |            |            |            |
| Cu(II)                              | 4.1        |            |            |            |
| Hf(IV)                              |            | 10.4       |            |            |
| Mo(VI)                              |            | 9.6        |            |            |
| Pb(II)                              | 6.0        |            |            |            |
| Th(IV)                              |            | 8.24       |            |            |
| UO <sub>2</sub> (II)                | 4.22       |            |            |            |
| V(V)                                |            | 8.6        |            |            |
| W(VI)                               |            | 7.8        |            |            |
| <b>Arsenazo</b>                     |            |            |            |            |
| Hf(IV)                              | 10.07      |            |            |            |
| Zr(IV)                              | 12.95      |            |            |            |
| <b>Aurintricarboxylic acid</b>      |            |            |            |            |
| Be(II)                              | 4.54       |            |            |            |
| Cu(II)                              | 4.1        | 8.81       |            |            |
| Fe(III)                             | 4.68       |            |            |            |
| Th(IV)                              | 5.04       |            |            |            |
| UO <sub>2</sub> (II)                | 4.77       |            |            |            |
| <b>Benzoylacetone (75% dioxane)</b> |            |            |            |            |
| Ba(II)                              |            | 9.4        |            |            |
| Be(II)                              | 12.59      | 24.01      |            |            |
| Cd(II)                              | 7.79       | 14.36      |            |            |
| Ce(III)                             | 10.09      | 19.42      | 27.04      |            |
| Co(II)                              | 9.42       | 17.83      |            |            |
| Cu(II)                              | 12.05      | 23.01      |            |            |
| La(III)                             | 6.33       | 11.66      | 16.78      |            |
| Mg(II)                              | 7.69       | 14.09      |            |            |
| Mn(II)                              | 8.66       | 15.78      |            |            |
| Ni(II)                              | 9.58       | 18.00      |            |            |
| Pb(II)                              | 8.84       | 16.35      |            |            |
| Pr(III)                             | 7.02       | 13.62      | 18.74      |            |
| UO <sub>2</sub> (II)                | 12.15      | 23.27      |            |            |
| Y(III)                              | 8.24       | 14.98      | 20.57      |            |
| Zn(II)                              | 9.62       | 17.90      |            |            |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                                                       |                            | log $K_1$    |           | log $K_2$                 |           | log $K_3$ |                     | log $K_4$ |           |  |
|-----------------------------------------------------------------------|----------------------------|--------------|-----------|---------------------------|-----------|-----------|---------------------|-----------|-----------|--|
| <b>Calmagite</b><br>Ca<br>Mg                                          |                            | 6.05<br>8.05 |           |                           |           |           |                     |           |           |  |
|                                                                       | Complex of $HL^{2-}$ Anion |              |           | Complex of $L^{3-}$ Anion |           |           | Complex of $H_2L^-$ |           |           |  |
|                                                                       | log $K_1$                  |              | log $K_2$ |                           | log $K_1$ |           | log $K_2$           |           | log $K_3$ |  |
| <b>Citric acid</b>                                                    |                            |              |           |                           |           |           |                     |           |           |  |
| Ag                                                                    | 7.1                        |              |           |                           |           |           |                     |           |           |  |
| Al                                                                    | 7.0                        |              |           | 20.0                      |           |           |                     |           |           |  |
| Ba                                                                    | 2.98                       |              |           |                           |           |           |                     |           |           |  |
| Be                                                                    | 4.52                       |              |           |                           |           |           |                     |           |           |  |
| Ca                                                                    | 4.68                       |              |           |                           |           |           |                     |           |           |  |
| Cd                                                                    | 3.98                       |              |           | 11.3                      |           |           |                     |           |           |  |
| Ce(III)                                                               |                            | 6.18         |           |                           | 9.65      |           |                     | 3.2       |           |  |
| Co(II)                                                                | 4.8                        |              |           | 12.5                      |           |           |                     |           |           |  |
| Cu(II)                                                                | 4.35                       |              |           | 14.2                      |           |           |                     |           |           |  |
| Eu(III)                                                               |                            | 6.46         |           |                           | 9.80      |           |                     |           |           |  |
| Fe(II)                                                                | 3.08                       |              |           | 15.5                      |           |           |                     |           |           |  |
| Fe(III)                                                               | 12.5                       |              |           | 25.0                      |           |           |                     |           |           |  |
| La                                                                    |                            | 6.97         |           |                           | 9.45      |           |                     | 6.22      |           |  |
| Mg                                                                    | 3.29                       |              |           |                           |           |           |                     |           |           |  |
| Mn(II)                                                                | 3.67                       |              |           |                           |           |           |                     |           |           |  |
| Nd(III)                                                               |                            | 6.32         |           |                           | 9.70      |           |                     |           |           |  |
| Ni                                                                    | 5.11                       |              |           | 14.3                      |           |           |                     |           |           |  |
| Pb                                                                    | 6.50                       |              |           |                           |           |           |                     |           |           |  |
| Pr                                                                    |                            |              |           |                           |           |           |                     | 3.4       |           |  |
| Ra                                                                    | 2.36                       |              |           |                           |           |           |                     |           |           |  |
| Sr                                                                    | 2.8                        |              |           |                           |           |           |                     |           |           |  |
| Tl(I)                                                                 | 1.04                       |              |           |                           |           |           |                     |           |           |  |
| UO <sub>2</sub>                                                       | 8.5                        | 10.8         |           |                           |           |           |                     |           |           |  |
| Y                                                                     |                            |              |           |                           |           |           |                     | 3.6       |           |  |
| Yb                                                                    |                            |              |           |                           | 8         |           |                     |           |           |  |
| Zn                                                                    | 4.71                       |              |           | 11.4                      |           |           |                     |           |           |  |
|                                                                       | log $K_1$                  |              | log $K_2$ |                           | log $K_3$ |           |                     |           |           |  |
| <b>1,2-Diaminocyclohexane-<math>N,N,N',N'</math>-tetraacetic acid</b> |                            |              |           |                           |           |           |                     |           |           |  |
| Al c                                                                  | 17.63                      |              |           |                           |           |           |                     |           |           |  |
| Ba c                                                                  | 8.64                       |              |           |                           |           |           |                     |           |           |  |
| Ca c                                                                  | 12.3                       |              |           |                           |           |           |                     |           |           |  |
| Cd c                                                                  | 19.88                      |              |           |                           |           |           |                     |           |           |  |
| Ce(III) c                                                             | 16.76                      |              |           |                           |           |           |                     |           |           |  |
| Co(II) c                                                              | 19.57                      |              |           |                           |           |           |                     |           |           |  |
| Cu(II) c                                                              | 21.95                      |              |           |                           |           |           |                     |           |           |  |
| Dy(III) c                                                             | 19.69                      |              |           |                           |           |           |                     |           |           |  |
| Er(III) c                                                             | 20.20                      |              |           |                           |           |           |                     |           |           |  |
| Eu(III) c                                                             | 18.77                      |              |           |                           |           |           |                     |           |           |  |
| Fe(III) c                                                             | 27.48                      |              |           |                           |           |           |                     |           |           |  |
| Ga c                                                                  | 22.91                      |              |           |                           |           |           |                     |           |           |  |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                                         | $\log K_1$ | $\log K_2$ | $\log K_3$ | $\log K_4$       |
|---------------------------------------------------------|------------|------------|------------|------------------|
| Gd <i>c</i>                                             | 18.80      |            |            |                  |
| Hg(II) <i>c</i>                                         | 24.4       |            |            |                  |
| Ho <i>c</i>                                             | 19.89      |            |            |                  |
| La <i>c</i>                                             | 16.35      |            |            |                  |
| Lu <i>c</i>                                             | 21.51      |            |            |                  |
| Mg <i>c</i>                                             | 10.41      |            |            |                  |
| Mn(II) <i>c</i>                                         | 17.43      |            |            |                  |
| Nd <i>c</i>                                             | 17.69      |            |            |                  |
| Ni <i>c</i>                                             | 19.4       |            |            |                  |
| Pb <i>c</i>                                             | 20.33      |            |            |                  |
| Pr <i>c</i>                                             | 17.23      |            |            |                  |
| Sm(III) <i>c</i>                                        | 18.63      |            |            |                  |
| Sr <i>c</i>                                             | 8.92       |            |            |                  |
| Tb <i>c</i>                                             | 19.30      |            |            |                  |
| Tm <i>c</i>                                             | 20.46      |            |            |                  |
| VO(II) <i>c</i>                                         | 19.40      |            |            |                  |
| Y <i>c</i>                                              | 19.41      |            |            |                  |
| Yb <i>c</i>                                             | 20.80      |            |            |                  |
| Zn <i>c</i>                                             | 18.6       |            |            |                  |
| <b>Dibenzoylmethane (75% dioxane)</b>                   |            |            |            |                  |
| Ba                                                      | 6.10       | 11.50      |            |                  |
| Be                                                      | 13.62      | 26.03      |            |                  |
| Ca                                                      | 7.17       | 13.55      |            |                  |
| Cd                                                      | 8.67       | 16.63      |            |                  |
| Ce(III)                                                 | 10.99      | 21.53      | 30.38      |                  |
| Co(II)                                                  | 10.35      | 20.05      |            |                  |
| Cu(II)                                                  | 12.98      | 24.98      |            |                  |
| Cs                                                      | 3.42       |            |            |                  |
| Fe(II)                                                  | 11.15      | 21.50      |            |                  |
| K                                                       | 3.67       |            |            |                  |
| Li                                                      | 5.95       |            |            |                  |
| Mg                                                      | 8.54       | 16.21      |            |                  |
| Mn(II)                                                  | 9.32       | 17.79      |            |                  |
| Na                                                      | 4.18       |            |            |                  |
| Ni                                                      | 10.83      | 20.72      |            |                  |
| Pb                                                      | 9.75       | 18.79      |            |                  |
| Rb                                                      | 3.52       |            |            |                  |
| Sr                                                      | 6.40       | 12.10      |            |                  |
| Zn                                                      | 10.23      | 19.65      |            |                  |
|                                                         | $\log K_1$ | $\log K_2$ | $\log K_3$ | $\log K_f$ [MHL] |
| <b>4,5-Dihydroxybenzene-1,3-disulfonic acid (Tiron)</b> |            |            |            |                  |
| Al                                                      | 19.02      | 31.10      | 33.5       |                  |
| Ba                                                      | 4.10       |            |            | 14.6             |
| Ca                                                      | 5.80       |            |            | 14.8             |
| Cd <i>d</i>                                             | 7.69       | 13.29      |            |                  |
| Ce(III)                                                 |            | 3.75       |            |                  |
| Co(II) <i>d</i>                                         | 8.19       | 14.41      |            | 15.7             |
| Cu(II) <i>d</i>                                         | 12.76      | 23.73      |            | 18.1             |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                        | log $K_1$      | log $K_2$ | log $K_3$                                  | log $K_f$ [MHL] |
|----------------------------------------|----------------|-----------|--------------------------------------------|-----------------|
| Fe(III) <i>a,c</i>                     | 20.7           | 35.9      | 46.9                                       | 22.6            |
| La                                     | 12.9           |           |                                            | 18.6 [La(OH)L]  |
| Mg <i>a,c</i>                          | 6.86           |           |                                            | 14.6            |
| Mn(II) <i>c</i>                        | 8.6            |           |                                            |                 |
| Ni <i>a,c</i>                          | 8.56           | 14.90     |                                            | 15.6            |
| Pb <i>d</i>                            | 11.95          | 18.28     |                                            |                 |
| Sr <i>c</i>                            | 4.55           |           |                                            |                 |
| UO <sub>2</sub> (II) <i>c</i>          | 15.90          |           |                                            |                 |
| VO(II)                                 | 15.88          |           |                                            |                 |
| Zn <i>d</i>                            | 9.00           | 16.91     |                                            | 15.9            |
|                                        | log $K_1$      | log $K_2$ | log $K_f$ [M <sub>2</sub> L <sub>3</sub> ] |                 |
| <b>2,3-Dimercaptopropan-1-ol (BAL)</b> |                |           |                                            |                 |
| Fe(II)                                 | 15.8           |           |                                            |                 |
| Fe(III)                                | 30.6 [Fe(OH)L] |           | 28                                         |                 |
| Mn(II)                                 | 5.23           | 10.43     |                                            |                 |
| Ni                                     |                | 22.78     |                                            |                 |
| Zn                                     | 13.48          | 23.3      | 40.6                                       |                 |
|                                        | log $K_1$      | log $K_2$ | log $K_3$                                  | log $K_4$       |
| <b>Dimethylglyoxime (50% dioxane)</b>  |                |           |                                            |                 |
| Cd                                     | 5.7            | 10.7      |                                            |                 |
| Co(II)                                 | 9.80           | 18.94     |                                            |                 |
| Cu(II)                                 | 12.00          | 33.44     |                                            |                 |
| Fe(II)                                 |                | 7.25      |                                            |                 |
| La                                     | 6.6            | 12.5      |                                            |                 |
| Ni                                     | 11.16          |           |                                            |                 |
| Pb                                     | 7.3            |           |                                            |                 |
| Zn                                     | 7.7            | 13.9      |                                            |                 |
| <b>2,2'-Dipyridyl</b>                  |                |           |                                            |                 |
| Ag                                     | 3.65           | 7.15      |                                            |                 |
| Cd                                     | 4.26           | 7.81      | 10.47                                      |                 |
| Co(II)                                 | 5.73           | 11.57     | 17.59                                      |                 |
| Cr(II)                                 | 4.5            | 10.5      | 14.0                                       |                 |
| Cu(I)                                  |                | 14.2      |                                            |                 |
| Cu(II)                                 | 8.0            | 13.60     | 17.08                                      |                 |
| Fe(II)                                 | 4.36           | 8.0       | 17.45                                      |                 |
| Hg(II)                                 | 9.64           | 16.74     | 19.54                                      |                 |
| Mg                                     | 0.5            |           |                                            |                 |
| Mn(II) <i>d</i>                        | 4.06           | 7.84      | 11.47                                      |                 |
| Ni                                     | 6.80           | 13.26     | 18.46                                      |                 |
| Pb                                     | 3.0            |           |                                            |                 |
| Ti(III)                                |                |           | 25.28                                      |                 |
| V(II)                                  | 4.9            | 9.6       | 13.1                                       |                 |
| Zn                                     | 5.30           | 9.83      | 13.63                                      |                 |
| <b>Eriochrome Black T</b>              |                |           |                                            |                 |
| Ca                                     | 5.4            |           |                                            |                 |
| Mg                                     | 7.0            |           |                                            |                 |
| Zn                                     | 13.5           | 20.6      |                                            |                 |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                                                                  | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$ |
|----------------------------------------------------------------------------------|-----------|-----------|-----------|-----------|
| <b>Ethanolamine</b>                                                              |           |           |           |           |
| Ag                                                                               | 3.29      | 6.92      |           | 16.48     |
| Cu(II)                                                                           |           | 6.68      |           |           |
| Hg(II)                                                                           | 8.51      | 17.32     |           |           |
| <b>Ethylenediamine</b>                                                           |           |           |           |           |
| Ag                                                                               | 4.70      | 7.70      |           |           |
| Cd <i>a</i>                                                                      | 5.47      | 10.09     | 12.09     |           |
| Co(II)                                                                           | 5.91      | 10.64     | 13.94     |           |
| Co(III)                                                                          | 18.7      | 34.9      | 48.69     |           |
| Cr(II)                                                                           | 5.15      | 9.19      |           |           |
| Cu(I)                                                                            |           | 10.8      |           |           |
| Cu(II)                                                                           | 10.67     | 20.00     | 21.0      |           |
| Fe(II)                                                                           | 4.34      | 7.65      | 9.70      |           |
| Hg(II)                                                                           | 14.3      | 23.3      |           |           |
| Mg                                                                               | 0.37      |           |           |           |
| Mn(II)                                                                           | 2.73      | 4.79      | 5.67      |           |
| Ni                                                                               | 7.52      | 13.84     | 18.33     |           |
| Pd(II)                                                                           |           | 26.90     |           |           |
| V(II)                                                                            | 4.6       | 7.5       | 8.8       |           |
| Zn                                                                               | 5.77      | 10.83     | 14.11     |           |
| <b>Ethylenediamine-<i>N</i>, <i>N</i>, <i>N'</i>, <i>N'</i>-tetraacetic acid</b> |           |           |           |           |
| Ag                                                                               | 7.32      |           |           |           |
| Al                                                                               | 16.11     |           |           |           |
| Am(III)                                                                          | 18.18     |           |           |           |
| Ba                                                                               | 7.78      |           |           |           |
| Be                                                                               | 9.3       |           |           |           |
| Bi                                                                               | 22.8      |           |           |           |
| Ca                                                                               | 11.0      |           |           |           |
| Cd                                                                               | 16.4      |           |           |           |
| Ce(III)                                                                          | 16.80     |           |           |           |
| Cf(III)                                                                          | 19.09     |           |           |           |
| Cm(III)                                                                          | 18.45     |           |           |           |
| Co(II)                                                                           | 16.31     |           |           |           |
| Co(III)                                                                          | 36        |           |           |           |
| Cr(II)                                                                           | 13.6      |           |           |           |
| Cr(III)                                                                          | 23        |           |           |           |
| Cu(II)                                                                           | 18.7      |           |           |           |
| Dy                                                                               | 18.0      |           |           |           |
| Er                                                                               | 18.15     |           |           |           |
| Eu(III)                                                                          | 17.99     |           |           |           |
| Fe(II)                                                                           | 14.33     |           |           |           |
| Fe(III)                                                                          | 24.23     |           |           |           |
| Ga                                                                               | 20.25     |           |           |           |
| Gd                                                                               | 17.2      |           |           |           |
| Hg(II)                                                                           | 21.80     |           |           |           |
| Ho                                                                               | 18.1      |           |           |           |
| In                                                                               | 24.95     |           |           |           |
| La                                                                               | 16.34     |           |           |           |
| Li                                                                               | 2.79      |           |           |           |
| Lu                                                                               | 19.83     |           |           |           |
| Mg                                                                               | 8.64      |           |           |           |
| Mn(II)                                                                           | 13.8      |           |           |           |
| Mo(V)                                                                            | 6.36      |           |           |           |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                    | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$ |
|--------------------|-----------|-----------|-----------|-----------|
| Na                 | 1.66      |           |           |           |
| Nd                 | 16.6      |           |           |           |
| Ni                 | 18.56     |           |           |           |
| Pb                 | 18.3      |           |           |           |
| Pd(II)             | 18.5      |           |           |           |
| Pm(III)            | 17.45     |           |           |           |
| Pr                 | 16.55     |           |           |           |
| Pu(III)            | 18.12     |           |           |           |
| Pu(IV)             | 17.66     |           |           |           |
| Pu(VI)             | 17.66     |           |           |           |
| Ra                 | 7.4       |           |           |           |
| Sc                 | 23.1      |           |           |           |
| Sm                 | 16.43     |           |           |           |
| Sn(II)             | 22.1      |           |           |           |
| Sr                 | 8.80      |           |           |           |
| Tb                 | 17.6      |           |           |           |
| Th                 | 23.2      |           |           |           |
| Ti(III)            | 21.3      |           |           |           |
| TiO(II)            | 17.3      |           |           |           |
| Tl(III)            | 22.5      |           |           |           |
| Tm                 | 19.49     |           |           |           |
| U(IV)              | 17.50     |           |           |           |
| V(II)              | 12.70     |           |           |           |
| V(III)             | 25.9      |           |           |           |
| VO(II)             | 18.0      |           |           |           |
| V(V)               | 18.05     |           |           |           |
| Y                  | 18.32     |           |           |           |
| Yb                 | 18.70     |           |           |           |
| Zn                 | 16.4      |           |           |           |
| Zr                 | 19.40     |           |           |           |
| <b>Glycine</b>     |           |           |           |           |
| Ag                 | 3.41      | 6.89      |           |           |
| Ba                 | 0.77      |           |           |           |
| Be                 |           | 4.95      |           |           |
| Ca                 | 1.38      |           |           |           |
| Cd                 | 4.74      | 8.60      |           |           |
| Co(II)             | 5.23      | 9.25      | 10.76     |           |
| Cu(II)             | 8.60      | 15.54     | 16.27     |           |
| Dy                 |           | 12.2      |           |           |
| Er                 |           | 12.7      |           |           |
| Fe(II) <i>a</i>    | 4.3       | 7.8       |           |           |
| Fe(III) <i>a,d</i> | 10.0      |           |           |           |
| Gd                 |           | 11.9      |           |           |
| Hg(II)             | 10.3      | 19.2      |           |           |
| La                 |           | 11.2      |           |           |
| Mg                 | 3.44      | 6.46      |           |           |
| Mn(II)             | 3.6       | 6.6       |           |           |
| Ni                 | 6.18      | 11.14     | 15        |           |
| Pb                 | 5.47      | 8.92      |           |           |
| Pd(II)             | 9.12      | 17.55     |           |           |
| Pr                 |           | 11.5      |           |           |
| Sm                 |           | 11.7      |           |           |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                                                               | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$ |
|-------------------------------------------------------------------------------|-----------|-----------|-----------|-----------|
| Sr                                                                            | 0.91      |           |           |           |
| Y                                                                             |           | 12.5      |           |           |
| Yb                                                                            |           | 13.0      |           |           |
| Zn                                                                            | 5.52      | 9.96      |           |           |
| <b><i>N'</i>-(2-Hydroxyethyl)ethylenediamine-<i>N,N,N'</i>-triacetic acid</b> |           |           |           |           |
| Ba <i>c</i>                                                                   | 5.54      |           |           |           |
| Ca <i>c</i>                                                                   | 8.43      |           |           |           |
| Cd <i>c</i>                                                                   | 13.0      |           |           |           |
| Ce(III) <i>c</i>                                                              | 14.11     |           |           |           |
| Co(II) <i>c</i>                                                               | 14.4      |           |           |           |
| Cu(II) <i>c</i>                                                               | 17.40     |           |           |           |
| Dy <i>c</i>                                                                   | 15.30     |           |           |           |
| Er <i>c</i>                                                                   | 15.42     |           |           |           |
| Eu(III) <i>c</i>                                                              | 15.35     |           |           |           |
| Fe(II) <i>c</i>                                                               | 11.6      |           |           |           |
| Fe(III) <i>c</i>                                                              | 19.8      |           |           |           |
| Gd <i>c</i>                                                                   | 15.22     |           |           |           |
| Hg(II) <i>c</i>                                                               | 20.1      |           |           |           |
| Ho <i>c</i>                                                                   | 15.32     |           |           |           |
| La <i>c</i>                                                                   | 13.46     |           |           |           |
| Lu <i>c</i>                                                                   | 15.88     |           |           |           |
| Mg <i>c</i>                                                                   | 5.78      |           |           |           |
| Mn(II) <i>c</i>                                                               | 10.7      |           |           |           |
| Nd <i>c</i>                                                                   | 14.86     |           |           |           |
| Ni <i>c</i>                                                                   | 17.0      |           |           |           |
| Pb <i>c</i>                                                                   | 15.5      |           |           |           |
| Pr <i>c</i>                                                                   | 14.61     |           |           |           |
| Sm <i>c</i>                                                                   | 15.28     |           |           |           |
| Sr <i>c</i>                                                                   | 6.92      |           |           |           |
| Tb <i>c</i>                                                                   | 15.32     |           |           |           |
| Th <i>c</i>                                                                   | 18.5      |           |           |           |
| Tm <i>c</i>                                                                   | 15.59     |           |           |           |
| Y <i>c</i>                                                                    | 14.65     |           |           |           |
| Yb <i>c</i>                                                                   | 15.88     |           |           |           |
| Zn <i>c</i>                                                                   | 14.5      |           |           |           |
| <b>8-Hydroxy-2-methylquinoline (50% dioxane)</b>                              |           |           |           |           |
| Cd                                                                            | 9.00      | 9.00      | 16.60     |           |
| Ce(III)                                                                       | 7.71      |           |           |           |
| Co(II)                                                                        | 9.63      | 18.50     |           |           |
| Cu(II)                                                                        | 12.48     | 24.00     |           |           |
| Fe(II)                                                                        | 8.75      | 17.10     |           |           |
| Mg                                                                            | 5.24      | 9.64      |           |           |
| Mn(II)                                                                        | 7.44      | 13.99     |           |           |
| Ni                                                                            | 9.41      | 17.76     |           |           |
| Pb                                                                            | 10.30     | 18.50     |           |           |
| UO <sub>2</sub> (II)                                                          | 9.4       | 17        |           |           |
| Zn                                                                            | 9.82      | 18.72     |           |           |
| <b>8-Hydroxyquinoline-5-sulfonic acid</b>                                     |           |           |           |           |
| Ba                                                                            | 2.31      |           |           |           |
| Ca                                                                            | 3.52      |           |           |           |
| Cd                                                                            | 7.70      | 14.20     |           |           |
| Ce(III)                                                                       | 6.05      | 11.05     | 14.95     |           |



**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                              | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$ |
|------------------------------|-----------|-----------|-----------|-----------|
| Co(II)                       | 8.11      | 15.05     | 20.41     | 32.04     |
| Cu(II)                       | 11.92     | 21.87     |           |           |
| Er                           | 7.16      | 13.34     | 18.56     |           |
| Fe(II)                       | 8.4       | 15.7      | 21.75     |           |
| Fe(III)                      | 11.6      | 22.8      | 35.65     |           |
| Gd                           | 6.64      | 12.37     | 17.27     |           |
| La                           | 5.63      | 10.13     | 13.83     |           |
| Mg                           | 4.79      | 8.19      |           |           |
| Mn(II)                       | 5.67      | 10.72     |           |           |
| Nd                           | 6.3       | 11.6      | 16.0      |           |
| Ni                           | 9.57      | 18.27     | 22.9      |           |
| Pb                           | 8.53      | 16.13     |           |           |
| Pr                           | 6.17      | 11.37     | 15.67     |           |
| Sm                           | 6.58      | 12.28     | 17.04     |           |
| Sr                           | 2.75      |           |           |           |
| Th                           | 9.56      | 18.29     | 25.92     |           |
| UO <sub>2</sub> (II)         | 8.52      | 15.67     |           |           |
| Zn                           | 8.65      | 16.15     |           |           |
| <b>Lactic acid</b>           |           |           |           |           |
| Ba                           | 0.64      |           |           |           |
| Ca                           | 1.42      |           |           |           |
| Cd                           | 1.70      |           |           |           |
| Ce(III) <i>a,c</i>           | 2.76      | 4.73      | 5.96      |           |
| Co(II)                       | 1.90      |           |           |           |
| Cu(II)                       | 3.02      | 4.85      |           |           |
| Er                           | 2.77      | 5.11      | 6.70      |           |
| Eu(III)                      | 2.53      | 4.60      | 5.88      |           |
| Fe(III)                      | 7.1       |           |           |           |
| Gd                           | 2.53      | 4.63      | 5.91      |           |
| Ho                           | 2.71      | 4.97      | 6.55      |           |
| La <i>a,c</i>                | 2.60      | 4.34      | 5.64      |           |
| Li                           | 0.20      |           |           |           |
| Mg                           | 1.37      |           |           |           |
| Mn(II)                       | 1.43      |           |           |           |
| Nd                           | 2.47      | 4.37      | 5.60      |           |
| Ni                           | 2.22      |           |           |           |
| Pb                           | 2.40      | 3.80      |           |           |
| Pr <i>a,c</i>                | 2.85      | 4.90      | 6.10      |           |
| Rare earths <i>a,c</i>       | 2.8–3.0   | 4.9–5.4   | 6.1–7.8   |           |
| Sm                           | 2.56      | 4.58      | 5.90      |           |
| Sr                           | 0.98      |           |           |           |
| Tb                           | 2.61      | 4.73      | 6.01      |           |
| Y                            | 2.53      | 4.70      | 6.12      |           |
| Yb                           | 2.85      | 5.27      | 7.96      |           |
| Zn                           | 2.20      | 3.75      |           |           |
| <b>Nitrilotriacetic acid</b> |           |           |           |           |
| Al                           | >10       |           |           |           |
| Ba <i>a</i>                  | 5.88      |           |           |           |
| Ca                           | 7.60      | 11.61     |           |           |
| Cd <i>c</i>                  | 9.80      | 15.2      |           |           |
| Ce(III) <i>c</i>             | 10.83     | 18.67     |           |           |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                           | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$                    |
|-------------------------------------------|-----------|-----------|-----------|------------------------------|
| Co(II) <i>c</i>                           | 10.38     | 14.5      |           |                              |
| Cr(III)                                   | >10       |           |           |                              |
| Cu(II) <i>c</i>                           | 13.10     |           |           |                              |
| Dy <i>c</i>                               | 11.74     | 21.15     |           |                              |
| Er <i>c</i>                               | 12.03     | 21.29     |           |                              |
| Eu(III) <i>c</i>                          | 11.52     | 20.70     |           |                              |
| Fe(II) <i>c</i>                           | 8.84      |           |           |                              |
| Fe(III) <i>c</i>                          | 15.87     | 24.32     |           |                              |
| Gd <i>c</i>                               | 11.54     | 20.80     |           |                              |
| Hg(II)                                    | 12.7      |           |           |                              |
| Ho <i>c</i>                               | 11.90     | 21.25     |           |                              |
| In                                        | 15        |           |           |                              |
| La <i>c</i>                               | 10.36     | 17.60     |           |                              |
| Li <i>a</i>                               | 3.28      |           |           |                              |
| Lu <i>c</i>                               | 12.49     | 21.91     |           |                              |
| Mg <i>c</i>                               | 5.36      | 10.2      |           |                              |
| Mn(II)                                    | 8.60      | 11.1      |           |                              |
| Na                                        | 2.15      |           |           |                              |
| Nd <i>c</i>                               | 11.26     | 19.73     |           |                              |
| Ni                                        | 11.26     | 16.0      |           |                              |
| Pb <i>a,c</i>                             | 11.8      |           |           |                              |
| Pr <i>c</i>                               | 11.07     | 19.25     |           |                              |
| Sm(III) <i>c</i>                          | 11.53     | 20.53     |           |                              |
| Sr                                        | 6.73      |           |           |                              |
| Tb <i>c</i>                               | 11.59     | 20.97     |           |                              |
| Tl(I)                                     | 3.44      |           |           |                              |
| Th <i>c</i>                               | 12.4      |           |           |                              |
| Tm <i>c</i>                               | 12.22     | 21.45     |           |                              |
| Y <i>c</i>                                | 11.48     | 20.43     |           |                              |
| Yb <i>c</i>                               | 12.40     | 21.69     |           |                              |
| Zn <i>c</i>                               | 10.45     | 13.45     |           |                              |
| Zr <i>c</i>                               | 20.8      |           |           |                              |
| <b>1-Nitroso-2-naphthol (75% dioxane)</b> |           |           |           |                              |
| Ag                                        | 7.74      |           |           |                              |
| Cd                                        | 6.18      | 11.38     |           |                              |
| Co(II)                                    | 10.67     | 22.81     |           |                              |
| Cu(II)                                    | 12.52     | 23.37     |           |                              |
| Mg                                        | 6.2       | 10.60     |           |                              |
| Nd                                        | 9.5       | 17.7      | 25.6      |                              |
| Ni                                        | 10.75     | 21.29     | 28.09     |                              |
| Pb                                        | 9.73      | 17.31     |           |                              |
| Pr                                        | 9.04      | 17.06     | 23.85     |                              |
| Th <i>c</i>                               | 8.50      | 16.13     | 24.03     | 30.29                        |
| Y                                         | 9.02      | 17.74     | 25.04     |                              |
| Zn                                        | 9.32      | 17.02     |           |                              |
| Zr                                        | 3.6       |           |           |                              |
| <b>Oxalate</b>                            |           |           |           |                              |
| Ag                                        | 2.41      |           |           |                              |
| Al                                        | 7.26      | 13.0      | 16.3      |                              |
| Am(III)                                   |           | 9.8       |           | [Am(HL) <sub>4</sub> ] 11.0] |
| Ba                                        | 2.31      |           |           |                              |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                            | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$                                 |
|----------------------------|-----------|-----------|-----------|-------------------------------------------|
| Be                         | 4.90      |           |           |                                           |
| Ca                         | 3.0       |           |           |                                           |
| Cd                         | 3.52      | 5.77      |           |                                           |
| Ce(III)                    | 6.52      | 10.5      | 11.3      |                                           |
| Co(II)                     | 4.79      | 6.7       | 9.7       |                                           |
| Co(III)                    |           |           | ~20       |                                           |
| Cu(II)                     | 6.16      | 8.5       |           |                                           |
| Er                         | 4.82      | 8.21      | 10.03     |                                           |
| Fe(II)                     | 2.9       | 4.52      | 5.22      |                                           |
| Fe(III)                    | 9.4       | 16.2      | 20.2      |                                           |
| Gd                         | 7.04      |           |           |                                           |
| Hg(II)                     |           | 6.98      |           |                                           |
| Mg                         | 3.43      | 4.38      |           |                                           |
| Mn(II)                     | 3.97      | 5.80      |           |                                           |
| Mn(III) <i>e</i>           | 9.98      | 16.57     | 19.42     |                                           |
| Mo(III)                    | 3.38      |           |           |                                           |
| Mo(VI)                     |           |           |           | [MoO <sub>3</sub> (L) <sup>2-</sup> 13.0] |
| Nd                         | 7.21      | 11.5      | > 14      |                                           |
| Ni                         | 5.3       | 7.64      | ~8.5      |                                           |
| NpO <sub>2</sub> (II)      | 3.30      | 7.07      |           |                                           |
| Pb                         |           | 6.54      |           |                                           |
| Pu(III)                    | 9.31      | 18.70     | 28        |                                           |
| Pu(IV)                     | 8.74      | 16.91     | 23.39     | 27.50                                     |
| PuO <sub>2</sub> (II)      |           | 11.4      |           |                                           |
| Sr                         | 2.54      |           |           |                                           |
| Th                         |           |           |           | 24.48                                     |
| TiO(II)                    | 2.67      |           |           |                                           |
| Tl(I)                      | 2.03      |           |           |                                           |
| UO <sub>2</sub> (II)       |           | 10.57     |           |                                           |
| VO(II)                     |           | 9.80      |           |                                           |
| V(II)                      | ~2.7      |           |           |                                           |
| Y                          | 6.52      | 10.10     | 11.47     |                                           |
| Yb                         | 7.30      | 11.7      | > 14      |                                           |
| Zn                         | 4.89      | 7.60      | 8.15      |                                           |
| Zr                         | 9.80      | 17.14     | 20.86     | 21.15                                     |
| <b>1,10-Phenanthroline</b> |           |           |           |                                           |
| Ag                         | 5.02      | 12.07     |           |                                           |
| Ca                         | 0.7       |           |           |                                           |
| Cd                         | 5.93      | 10.53     | 14.31     |                                           |
| Co(II)                     | 7.25      | 13.95     | 19.90     |                                           |
| Cu(II)                     | 9.08      | 15.76     | 20.94     |                                           |
| Fe(II)                     | 5.85      | 11.45     | 21.3      |                                           |
| Fe(III)                    | 6.5       | 11.4      | 23.5      |                                           |
| Hg(II)                     |           | 19.65     | 23.35     |                                           |
| Mg                         | 1.2       |           |           |                                           |
| Mn(II)                     | 3.88      | 7.04      | 10.11     |                                           |
| Ni                         | 8.80      | 17.10     | 24.80     |                                           |
| Pb                         | 4.65      | 7.5       | 9         |                                           |
| VO(II)                     | 5.47      | 9.69      |           |                                           |
| Zn                         | 6.55      | 12.35     | 17.55     |                                           |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                       | $\log K_1$ | $\log K_2$ | $\log K_3$      | $\log K_4$      |
|---------------------------------------|------------|------------|-----------------|-----------------|
| <b>Phthalic acid</b>                  |            |            |                 |                 |
| Ba                                    | 2.33       |            |                 |                 |
| Ca                                    | 2.43       |            |                 |                 |
| Cd                                    | 2.5        |            |                 |                 |
| Co(II)                                | 1.81       | 4.51       |                 |                 |
| Cu(II)                                | 3.46       | 4.83       |                 |                 |
| La                                    |            | 7.74       |                 |                 |
| Ni                                    | 2.14       |            |                 |                 |
| Pb <i>d</i>                           | 3.4        |            |                 |                 |
| UO <sub>2</sub> (II)                  | 4.38       |            |                 |                 |
| Zn                                    | 2.2        |            |                 |                 |
| <b>Piperidine</b>                     |            |            |                 |                 |
| Ag                                    | 3.30       | 6.48       |                 |                 |
| Hg(II)                                | 8.70       | 17.44      |                 |                 |
| Pt(II)                                |            |            | $\log K_5$ 5.7  | $\log K_6$ 8.2  |
| <b>Propylene-1,2-diamine</b>          |            |            |                 |                 |
| Cd <i>b,c</i>                         |            | 9.97       | 12.12           |                 |
| Co(II) <i>d</i>                       | 5.42       | 11.47      | 14.72           |                 |
| Cu(II) <i>c</i>                       | 6.41       | 20.06      |                 |                 |
| Hg(II) <i>c</i>                       | 10.78      | 23.53      | 23.25           |                 |
| Ni <i>d</i>                           | 7.43       | 13.62      | 17.89           |                 |
| Zn <i>b,c</i>                         | 5.89       | 10.87      | 12.57           |                 |
| <b>Pyridine</b>                       |            |            |                 |                 |
| Ag                                    | 1.97       | 4.35       |                 |                 |
| Cd                                    | 1.40       | 1.95       | 2.27            | 2.50            |
| Co(II)                                | 1.14       | 1.54       |                 |                 |
| Cu(I)                                 |            | 3.34       | 4.51            | 5.44            |
| Cu(II)                                | 2.59       | 4.33       | 5.93            | $\log K_6$ 6.89 |
| Fe(II)                                | 0.71       |            | $\log K_5$ 7.00 | 6.54            |
| Hg(II)                                | 5.1        | 10.0       | 10.4            | $\log K_6$ 10.2 |
| Mn(II)                                | 1.92       | 2.77       | 3.37            | 3.50            |
| VO(II)                                | -1.70      |            |                 |                 |
| Zn                                    | 1.41       | 1.11       | 1.61            | 1.93            |
| <b>Pyridine-2,6-dicarboxylic acid</b> |            |            |                 |                 |
| Ba <i>a,d</i>                         | 3.46       |            |                 |                 |
| Ca <i>a,d</i>                         | 4.6        | 7.2        |                 |                 |
| Cd <i>a,d</i>                         | 5.7        | 10.0       |                 |                 |
| Ce(III) <i>a,d</i>                    | 8.34       | 14.42      | 18.80           |                 |
| Co(II) <i>a,d</i>                     | 7.0        | 12.5       |                 |                 |
| Cu(II) <i>a,d</i>                     | 9.14       | 16.52      |                 |                 |
| Dy <i>a,d</i>                         | 8.69       | 16.19      | 22.14           |                 |
| Er <i>a,d</i>                         | 8.77       | 16.39      | 22.14           |                 |
| Eu(III) <i>a,d</i>                    | 8.84       | 15.98      | 21.00           |                 |
| Fe(II) <i>a,d</i>                     | 5.71       | 10.36      |                 |                 |
| Fe(III) <i>a,d</i>                    | 10.91      | 17.13      |                 |                 |
| Gd <i>a,d</i>                         | 8.74       | 16.06      | 21.83           |                 |
| Ho <i>a,d</i>                         | 8.72       | 16.23      | 22.08           |                 |
| La <i>a,d</i>                         | 7.98       | 13.79      | 18.06           |                 |
| Lu <i>a,d</i>                         | 9.03       | 16.80      | 21.48           |                 |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                                    | log $K_1$ | log $K_2$      | log $K_3$                    | log $K_4$                       |
|----------------------------------------------------|-----------|----------------|------------------------------|---------------------------------|
| Hg(II) <i>a,d</i>                                  | 20.28     |                |                              |                                 |
| Mg <i>a,d</i>                                      | 2.7       |                |                              |                                 |
| Mn(II) <i>a,d</i>                                  | 5.01      | 8.49           |                              |                                 |
| Nd <i>a,d</i>                                      | 8.78      | 15.60          | 20.66                        |                                 |
| Ni <i>a,d</i>                                      | 6.95      | 13.50          |                              |                                 |
| Pb <i>a,d</i>                                      | 8.70      | 10.60          |                              |                                 |
| Pr <i>a,d</i>                                      | 8.63      | 15.10          | 19.94                        |                                 |
| Sm <i>a,d</i>                                      | 8.86      | 15.88          | 21.23                        |                                 |
| Sr <i>a,d</i>                                      | 3.89      |                |                              |                                 |
| Tb <i>a,d</i>                                      | 8.68      | 16.11          | 22.03                        |                                 |
| Tm <i>a,d</i>                                      | 8.83      | 16.54          | 22.04                        |                                 |
| Y <i>a,d</i>                                       | 8.46      | 15.73          | 21.34                        |                                 |
| Yb <i>a,d</i>                                      | 8.85      | 16.61          | 21.83                        |                                 |
| Zn <i>a,d</i>                                      | 6.35      | 11.88          |                              |                                 |
| 1-(2-Pyridylazo)-2-naphthol (PAN)                  |           |                |                              |                                 |
| Co(II)                                             | > 12      |                |                              |                                 |
| Cu(II)                                             | 16        |                |                              |                                 |
| Mn(II)                                             | 8.5       | 16.4           |                              |                                 |
| Ni                                                 | 12.7      | 25.3           |                              |                                 |
| Tl(III)                                            | 2.29      |                |                              |                                 |
| Zn                                                 | 11.2      | 21.7           |                              |                                 |
|                                                    |           | log $K_f$ [ML] | log $K_f$ [MHL]              | log $K_f$ [M(HL) <sub>2</sub> ] |
| 4-(2-Pyridylazo)resorcinal (PAR)                   |           |                |                              |                                 |
| Co(II)                                             |           |                | > 12                         |                                 |
| Cu(II)                                             | 10.3      |                |                              |                                 |
| Mn(II)                                             |           |                | 9.7                          | 18.9                            |
| Ni                                                 |           |                | 13.2                         | 26.0                            |
| Sc                                                 | 4.8       |                |                              |                                 |
| Tl(III)                                            | 4.23      |                |                              |                                 |
| Zn                                                 |           |                | 12.4                         | 23.5                            |
|                                                    |           | log $K_f$ [ML] | log $K_f$ [M <sub>2</sub> L] | log $K_f$ [MHL]                 |
| Pyrocatechol-3,5-disulfonate (Pyrocatechol Violet) |           |                |                              |                                 |
| Al                                                 | 19.13     |                | 4.95                         |                                 |
| Bi                                                 | 27.07     |                | 5.25                         |                                 |
| Cd                                                 | 8.13      |                |                              | 5.86                            |
| Co(II)                                             | 9.01      |                |                              | 6.53                            |
| Cu(II)                                             | 16.47     |                |                              | 11.18                           |
| Ga                                                 | 22.18     | 4.65           |                              |                                 |
| In                                                 | 18.10     | 4.81           |                              |                                 |
| Mg                                                 | 4.42      | 4.6            |                              | 3.66                            |
| Mn(II)                                             | 7.13      |                |                              | 5.36                            |
| Ni                                                 | 9.35      | 4.38           |                              | 6.85                            |
| Pb                                                 | 13.25     |                |                              | 10.19                           |
| Th                                                 | 23.36     | 4.42           |                              |                                 |
| Zn                                                 | 10.41     | 6.21           |                              | 7.21                            |
| Zr                                                 | 27.40     | 4.18           |                              |                                 |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                    | $\log K_1$                | $\log K_2$ | $\log K_3$                         | $\log K_4$ |
|------------------------------------|---------------------------|------------|------------------------------------|------------|
| <b>8-Quinolinol</b>                |                           |            |                                    |            |
| Ba                                 | 2.07                      |            |                                    |            |
| Be                                 | 3.36                      |            |                                    |            |
| Ca (75% dioxane)                   | 7.3                       | 13.2       |                                    |            |
| Cd                                 | 7.2                       | 13.4       |                                    |            |
| Ce(III) (50% dioxane)              | 9.15                      | 17.13      |                                    |            |
| Co(II)                             | 9.1                       | 17.2       |                                    |            |
| Cu(II)                             | 12.2                      | 23.4       |                                    |            |
| Fe(II)                             | 8.58                      | 16.93      | 22.23                              |            |
| Fe(III)                            | 12.3                      | 23.6       | 33.9                               |            |
| La                                 | 5.85                      | 16.95      |                                    |            |
| Mg (50% dioxane)                   | 6.38                      | 11.81      |                                    |            |
| Mn(II) (50% dioxane)               | 8.28                      | 15.45      |                                    |            |
| Ni (50% dioxane)                   | 11.44                     | 21.38      |                                    |            |
| Pb (50% dioxane)                   | 10.61                     | 18.70      |                                    |            |
| Sm                                 | 6.84                      |            | 19.50                              |            |
| Sr                                 | 2.89                      | 6.08       |                                    |            |
| Th                                 | 10.45                     | 20.40      | 29.85                              | 38.80      |
| UO <sub>2</sub> (II) (50% dioxane) | 11.25                     | 20.89      |                                    |            |
| V(II)                              | 12.8                      | 23.6       |                                    |            |
| VO(II)                             | 10.97                     | 20.19      |                                    |            |
| Y                                  | 8.15                      | 14.90      | 20.25                              |            |
| Zn (50% dioxane)                   | 9.96                      | 18.86      |                                    |            |
|                                    | $\log K_f [\text{MHL}^+]$ |            | $\log K_f [\text{M}(\text{HL})_2]$ |            |
| <b>Salicylaldoxime</b>             |                           |            |                                    |            |
| Ba                                 | 0.53                      |            |                                    | 3.72       |
| Be                                 | <7                        |            |                                    |            |
| Ca                                 | 0.92                      |            |                                    | 3.72       |
| Cd                                 | <4.4                      |            |                                    |            |
| Co(II)                             |                           |            |                                    | 8.13       |
| Cu(II)                             |                           |            |                                    | 8.13       |
| Mg                                 | 0.64                      |            |                                    | 4.10       |
| Ni                                 |                           |            |                                    | 3.77       |
| Sr                                 |                           |            |                                    | 3.77       |
| Zn                                 | <5.2                      |            |                                    |            |
|                                    | $\log K_1$                | $\log K_2$ | $\log K_3$                         | $\log K_4$ |
| <b>Salicylic acid</b>              |                           |            |                                    |            |
| Al                                 | 14.11                     |            |                                    |            |
| Be                                 | 17.4                      |            |                                    |            |
| Cd                                 | 5.55                      |            |                                    |            |
| Ce(III)                            | 2.66                      |            |                                    |            |
| Co(II)                             | 6.72                      | 11.42      |                                    |            |
| Cr(II)                             | 8.4                       | 15.3       |                                    |            |
| Cu(II)                             | 10.60                     | 18.45      |                                    |            |
| Fe(II)                             | 6.55                      | 11.25      |                                    |            |
| Fe(III) <i>a,c</i>                 | 16.48                     | 28.12      | 36.80                              |            |
| La                                 | 2.64                      |            |                                    |            |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                              | log $K_1$ | log $K_2$ | log $K_3$ | log $K_4$                                              |
|------------------------------|-----------|-----------|-----------|--------------------------------------------------------|
| Mg (75% dioxane)             | 4.7       |           |           |                                                        |
| Mn(II)                       | 5.90      | 9.80      |           |                                                        |
| Nd                           | 2.70      |           |           |                                                        |
| Ni                           | 6.95      | 11.75     |           |                                                        |
| Pr                           | 2.68      |           |           |                                                        |
| Th                           | 4.25      | 7.60      | 10.05     | 11.60                                                  |
| TiO(II)                      | 6.09      |           |           |                                                        |
| UO <sub>2</sub> (II)         | 13.4      |           |           |                                                        |
| V(II)                        | 6.3       |           |           |                                                        |
| Zn                           | 6.85      |           |           |                                                        |
| <b>Succinic acid</b>         |           |           |           |                                                        |
| Ba                           | 2.08      |           |           |                                                        |
| Be                           | 3.08      |           |           |                                                        |
| Ca                           | 2.0       |           |           |                                                        |
| Cd                           | 2.2       |           |           |                                                        |
| Co(II)                       | 2.22      |           |           |                                                        |
| Cu(II)                       | 3.33      |           |           |                                                        |
| Fe(III)                      | 7.49      |           |           |                                                        |
| Hg(II)                       |           | 7.28      |           |                                                        |
| La                           | 3.96      |           |           |                                                        |
| Mg                           | 1.20      |           |           |                                                        |
| Mn(II)                       | 2.26      |           |           |                                                        |
| Nd                           | 8.1       |           |           |                                                        |
| Ni                           | 2.36      |           |           |                                                        |
| Pb                           | 2.8       |           |           |                                                        |
| Ra                           | 1.0       |           |           |                                                        |
| Sr                           | 1.06      |           |           |                                                        |
| Zn                           | 1.6       |           |           |                                                        |
| <b>5-Sulfosalicylic acid</b> |           |           |           |                                                        |
| Al c                         | 13.20     | 22.83     | 28.89     |                                                        |
| Be c                         | 11.71     | 20.81     |           |                                                        |
| Cd c                         | 16.68     | 29.08     |           |                                                        |
| Co(II) c                     | 6.13      | 9.82      |           |                                                        |
| Cr(II) c                     | 7.1       | 12.9      |           |                                                        |
| Cr(III) c                    | 9.56      |           |           |                                                        |
| Cu(II) c                     | 9.52      | 16.45     |           |                                                        |
| Fe(II) c                     | 5.90      |           |           |                                                        |
| Fe(III) c                    | 14.64     | 25.18     | 32.12     |                                                        |
| La c                         | 9.11      |           |           |                                                        |
| Mn(II) c                     | 5.24      | 8.24      |           |                                                        |
| NbO(III) c                   | 4.0       | 7.7       |           |                                                        |
| Ni c                         | 6.42      | 10.24     |           |                                                        |
| UO <sub>2</sub> (II) c       | 11.14     | 19.20     |           |                                                        |
| Zn c                         | 6.05      | 10.65     |           |                                                        |
| <b>Tartaric acid</b>         |           |           |           |                                                        |
| Ba                           |           | 1.62      |           |                                                        |
| Bi                           |           |           | 8.30      |                                                        |
| Ca                           | 2.98      | 9.01      |           |                                                        |
| Cd                           | 2.8       |           |           |                                                        |
| Co(II)                       | 2.1       |           |           |                                                        |
| Cu(II)                       | 3.2       | 5.11      | 4.78      | 6.51                                                   |
|                              |           |           |           | log $K_f$ 19.14 [Cu(OH) <sub>2</sub> L <sup>2-</sup> ] |

**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                     | $\log K_1$ | $\log K_2$ | $\log K_3$ | $\log K_4$                                             |
|-------------------------------------|------------|------------|------------|--------------------------------------------------------|
| Eu(III)                             | 4.98       | 8.11       |            |                                                        |
| Fe(III)                             | 7.49       |            |            |                                                        |
| La                                  | 3.06       |            |            |                                                        |
| Mg                                  |            | 1.36       |            |                                                        |
| Nd                                  | 9.0        |            |            |                                                        |
| Pb                                  | 3.78       |            | 4.7        | $\log K_f$ 14.1 [Pb(OH) <sub>2</sub> L <sup>2-</sup> ] |
| Ra                                  | 1.24       |            |            |                                                        |
| Sr                                  | 1.60       |            |            |                                                        |
| Zn                                  | 2.68       | 8.32       |            |                                                        |
| <b>Thioglycolic acid</b>            |            |            |            |                                                        |
| Ce(III) <i>a,c</i>                  | 1.99       | 3.03       |            |                                                        |
| Co(II)                              | 5.84       | 12.15      |            |                                                        |
| Fe(II)                              |            | 10.92      |            |                                                        |
| Hg(II)                              |            | 43.82      |            |                                                        |
| La <i>a,c</i>                       | 1.98       | 2.98       |            |                                                        |
| Mn(II)                              | 4.38       | 7.56       |            |                                                        |
| Pb                                  | 8.5        |            |            |                                                        |
| Ni                                  | 6.98       | 13.53      |            |                                                        |
| Rare earths <i>a,c</i>              | 1.9–2.1    | 3.0–3.3    |            |                                                        |
| Y <i>a,c</i>                        | 1.91       | 3.19       |            |                                                        |
| Zn                                  | 7.86       | 15.04      |            |                                                        |
| <b>Thiourea</b>                     |            |            |            |                                                        |
| Ag                                  | 7.4        | 13.1       |            |                                                        |
| Bi                                  |            |            |            | $\log K_6$ 11.9                                        |
| Cd                                  | 0.6        | 1.6        | 2.6        | 4.6                                                    |
| Cu(I)                               |            |            | 13         | 15.4                                                   |
| Hg(II)                              |            | 22.1       | 24.7       | 26.8                                                   |
| Pb                                  | 1.4        | 3.1        | 4.7        | 8.3                                                    |
| Ru(III)                             | 1.21       |            | 0.72       |                                                        |
| <b>Thoron</b>                       |            |            |            |                                                        |
| Th                                  |            | 10.15      |            |                                                        |
| <b>Triethanolamine</b>              |            |            |            |                                                        |
| Ag                                  | 2.30       | 3.64       |            |                                                        |
| Co(II)                              | 1.73       |            |            |                                                        |
| Cu(II)                              | 4.30       |            |            |                                                        |
| Hg(II)                              | 6.90       | 13.08      |            |                                                        |
| Ni                                  | 2.7        |            |            |                                                        |
| Zn                                  | 2.00       |            |            |                                                        |
| <b>Triethylenetetramine (Trien)</b> |            |            |            |                                                        |
| Ag                                  | 7.7        |            |            |                                                        |
| Cd                                  | 10.75      | 13.9       |            |                                                        |
| Co(II)                              | 11.0       |            |            |                                                        |
| Cu(II)                              | 20.4       |            |            |                                                        |
| Fe(II)                              | 7.8        |            |            |                                                        |
| Fe(III)                             | 21.9       |            |            |                                                        |
| Hg(II)                              | 25.26      |            |            |                                                        |
| Mn(II)                              | 4.9        |            |            |                                                        |
| Ni                                  | 14.0       |            |            |                                                        |
| Pb                                  | 10.4       |            |            |                                                        |
| Zn                                  | 11.9       |            |            |                                                        |



**TABLE 8.13** Cumulative Formation Constants for Metal Complexes with Organic Ligands (*Continued*)

|                                                  | log $K_1$             | log $K_2$ | log $K_3$ | log $K_4$ |
|--------------------------------------------------|-----------------------|-----------|-----------|-----------|
| <b>1,1,1-Trifluoro-3-2'-Thenoylacetone (TTA)</b> |                       |           |           |           |
| Ba                                               |                       | 10.6      |           |           |
| Cu(II)                                           | 6.55                  | 13.0      |           |           |
| Fe(III)                                          | 6.9                   |           |           |           |
| Ni                                               | 10.0                  |           |           |           |
| Pr                                               | 9.53                  |           |           |           |
| Pu(III)                                          | 9.53                  |           |           |           |
| Pu(IV)                                           | 8.0                   |           |           |           |
| Th                                               | 8.1                   |           |           |           |
| U(IV)                                            | 7.2                   |           |           |           |
| Zr                                               | 3.03 [as $ZrL^{3+}$ ] |           |           |           |
| <b>Xylenol orange</b>                            |                       |           |           |           |
| Bi                                               | 5.52                  |           |           |           |
| Fe(III)                                          | 5.70                  |           |           |           |
| Hf                                               | 6.50                  |           |           |           |
| Tl(III)                                          | 4.90                  |           |           |           |
| Zn                                               | 6.15                  |           |           |           |
| Zr                                               | 7.60                  |           |           |           |
| <b>Zincon</b>                                    |                       |           |           |           |
| Zn                                               | 13.1                  |           |           |           |

8.3 BUFFER SOLUTIONS

8.3.1 Standard Reference pH Buffer Solutions

The assigned values of  $pH_s$ , according to the Bates-Guggenheim convention [*Pure Applied Chem.* 1:163 (1960)], for the primary standard solutions prepared from salts issued by the National Institute for Science and Technology (NIST, US) (U.S.) are given in Table 8.14. These are smoothed values. The ionic strength of these reference solutions is 0.1 or less. Strictly speaking the NIST scale uses a molality concentration system; however, values are given in molarity units for convenience.

As a result of a variable liquid-junction potential, the measured pH may be expected to differ seriously from the  $pa_H$  determined from cells without a liquid junction in solutions of high acidity or high alkalinity. Merely to affirm the proper functioning of the glass electrode at the extreme ends of the pH scale, two secondary standards are included in Table 8.14. In addition, values for a 0.1 *m* solution of HCl are given to extend the pH scale up to 275°C [see R. S. Greeley, *Anal. Chem.* 32:1717 (1960)]:

|                |      |      |      |      |      |      |      |         |
|----------------|------|------|------|------|------|------|------|---------|
| $t, ^\circ C:$ | 25   | 60   | 90   | 125  | 150  | 175  | 200  | 225–275 |
| pH:            | 1.10 | 1.11 | 1.12 | 1.13 | 1.14 | 1.15 | 1.16 | 1.2     |

Uncertainties in the values are  $\pm 0.03$  pH unit from 25 to 90°C,  $\pm 0.05$  pH unit from 125 to 200°C, and  $\pm 0.1$  pH unit from 225 to 275°C.

**TABLE 8.14** National Bureau of Standards (U.S.) Reference pH Buffer Solutions

| Temperature<br>°C                    | Secondary<br>standard<br>0.05 M<br>K<br>tetraoxalate | KH tartrate<br>(saturated at 25°C) | 0.05 M<br>KH <sub>2</sub><br>citrate | 0.05 M<br>KH<br>phthalate | 0.025 M<br>KH <sub>2</sub> PO <sub>4</sub> ,<br>0.025 M<br>Na <sub>2</sub> HPO <sub>4</sub> | 0.0087 M<br>KH <sub>2</sub> PO <sub>4</sub> ,<br>0.0302 M<br>Na <sub>2</sub> HPO <sub>4</sub> | 0.01 M<br>Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> | 0.025 M<br>NaHCO <sub>3</sub> ,<br>0.025 M<br>Na <sub>2</sub> CO <sub>3</sub> | Secondary<br>standard Ca(OH) <sub>2</sub><br>(saturated at 25°C) |
|--------------------------------------|------------------------------------------------------|------------------------------------|--------------------------------------|---------------------------|---------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|---------------------------------------------------------|-------------------------------------------------------------------------------|------------------------------------------------------------------|
| 0                                    | 1.666                                                |                                    | 3.860                                | 4.003                     | 6.984                                                                                       | 7.534                                                                                         | 9.464                                                   | 10.317                                                                        | 13.423                                                           |
| 5                                    | 1.668                                                |                                    | 3.840                                | 3.999                     | 6.951                                                                                       | 7.500                                                                                         | 9.395                                                   | 10.245                                                                        | 13.207                                                           |
| 10                                   | 1.638                                                |                                    | 3.820                                | 3.997                     | 6.923                                                                                       | 7.472                                                                                         | 9.332                                                   | 10.179                                                                        | 13.003                                                           |
| 15                                   | 1.642                                                |                                    | 3.802                                | 3.998                     | 6.900                                                                                       | 7.448                                                                                         | 9.276                                                   | 10.118                                                                        | 12.810                                                           |
| 20                                   | 1.644                                                |                                    | 3.788                                | 4.002                     | 6.881                                                                                       | 7.429                                                                                         | 9.225                                                   | 10.062                                                                        | 12.627                                                           |
| 25                                   | 1.646                                                | 3.557                              | 3.776                                | 4.005                     | 6.865                                                                                       | 7.413                                                                                         | 9.180                                                   | 10.012                                                                        | 12.454                                                           |
| 30                                   | 1.648                                                | 3.552                              | 3.766                                | 4.011                     | 6.853                                                                                       | 7.400                                                                                         | 9.139                                                   | 9.966                                                                         | 12.289                                                           |
| 35                                   |                                                      | 3.549                              | 3.759                                | 4.018                     | 6.844                                                                                       | 7.389                                                                                         | 9.102                                                   | 9.925                                                                         | 12.133                                                           |
| 38                                   | 1.649                                                | 3.548                              | 3.756                                | 4.030                     | 6.840                                                                                       | 7.384                                                                                         | 9.088                                                   | 9.910                                                                         | 12.043                                                           |
| 40                                   | 1.650                                                | 3.547                              | 3.753                                | 4.035                     | 6.838                                                                                       | 7.380                                                                                         | 9.068                                                   | 9.889                                                                         | 11.984                                                           |
| 45                                   |                                                      | 3.547                              |                                      | 4.047                     | 6.834                                                                                       | 7.373                                                                                         | 9.038                                                   |                                                                               | 11.841                                                           |
| 50                                   | 1.653                                                | 3.549                              | 3.749                                | 4.050                     | 6.833                                                                                       | 7.367                                                                                         | 9.011                                                   | 9.828                                                                         | 11.705                                                           |
| 55                                   |                                                      | 3.554                              |                                      | 4.075                     | 6.834                                                                                       |                                                                                               | 8.985                                                   |                                                                               | 11.574                                                           |
| 60                                   | 1.660                                                | 3.560                              |                                      | 4.081                     | 6.836                                                                                       |                                                                                               | 8.962                                                   |                                                                               | 11.449                                                           |
| 70                                   | 1.671                                                | 3.580                              |                                      | 4.116                     | 6.845                                                                                       |                                                                                               | 8.921                                                   |                                                                               |                                                                  |
| 80                                   | 1.689                                                | 3.609                              |                                      | 4.164                     | 6.859                                                                                       |                                                                                               | 8.885                                                   |                                                                               |                                                                  |
| 90                                   | 1.72                                                 | 3.650                              |                                      | 4.205                     | 6.877                                                                                       |                                                                                               | 8.850                                                   |                                                                               |                                                                  |
| 95                                   | 1.73                                                 | 3.674                              |                                      | 4.227                     | 6.886                                                                                       |                                                                                               | 8.833                                                   |                                                                               |                                                                  |
| Dilution value<br>ΔpH <sub>1/2</sub> | +0.186                                               | +0.049                             | 0.024                                | +0.052                    | +0.080                                                                                      | +0.070                                                                                        | +0.01                                                   | 0.079                                                                         | −0.28                                                            |

**Source:** R. G. Bates, *J. Res. Natl. Bur. Stand. (U.S.)*, **66A**:179 (1962) and B. R. Staples and R. G. Bates, *J. Res. Natl. Bur. Stand. (U.S.)*, **73A**:37 (1969).

**Note:** The uncertainty is ±0.003 in pH in the range 0–50°C, rising to ±0.02 above 70°C.

**TABLE 8.15** Compositions of Standard pH Buffer Solutions [National Bureau of Standards (U.S.)]  
*Air weight of material per liter of buffer solution.*

| Standard                                                                        | Weight, g         |
|---------------------------------------------------------------------------------|-------------------|
| $\text{KH}_2(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$ , 0.05 <i>M</i> | 12.61             |
| Potassium hydrogen tartrate, about 0.034 <i>M</i>                               | Saturated at 25°C |
| Potassium hydrogen phthalate, 0.05 <i>M</i>                                     | 10.12             |
| Phosphate:                                                                      |                   |
| $\text{KH}_2\text{PO}_4$ , 0.025 <i>M</i>                                       | 3.39              |
| $\text{Na}_2\text{HPO}_4$ , 0.025 <i>M</i>                                      | 3.53              |
| Phosphate:                                                                      |                   |
| $\text{KH}_2\text{PO}_4$ , 0.008665 <i>M</i>                                    | 1.179             |
| $\text{Na}_2\text{HPO}_4$ , 0.03032 <i>M</i>                                    | 4.30              |
| $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$ , 0.01 <i>M</i>    | 3.80              |
| Carbonate:                                                                      |                   |
| $\text{NaHCO}_3$ , 0.025 <i>M</i>                                               | 2.10              |
| $\text{Na}_2\text{CO}_3$ , 0.025 <i>M</i>                                       | 2.65              |
| $\text{Ca}(\text{OH})_2$ , about 0.0203 <i>M</i>                                | Saturated at 25°C |

The buffer values for the NBS reference pH buffer solutions are given below:

|                 |          | 0.05 <i>M</i>   | 0.05 <i>M</i> | 0.025 <i>M</i>                    | 0.0087 <i>M</i>                   |                                               | 0.025 <i>M</i>                  |
|-----------------|----------|-----------------|---------------|-----------------------------------|-----------------------------------|-----------------------------------------------|---------------------------------|
|                 | KH       | KH <sub>2</sub> | KH            | KH <sub>2</sub> PO <sub>4</sub> , | KH <sub>2</sub> PO <sub>4</sub> , |                                               | NaHCO <sub>3</sub> ,            |
| Buffer solution | tartrate | citrate         | phthalate     | 0.25 <i>M</i>                     | 0.0302 <i>M</i>                   | 0.01 <i>M</i>                                 | 0.025 <i>M</i>                  |
|                 |          |                 |               | Na <sub>2</sub> HPO <sub>4</sub>  | Na <sub>2</sub> HPO <sub>4</sub>  | Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> | Na <sub>2</sub> CO <sub>3</sub> |
| Buffer value β  | 0.027    | 0.034           | 0.016         | 0.029                             | 0.016                             | 0.020                                         | 0.029                           |

For the secondary pH reference standards, the buffer value is 0.070 for potassium tetroxalate and 0.09 for calcium hydroxide.

To prepare the standard pH buffer solutions recommended by the National Bureau of Standards (U.S.), the indicated weights of the pure materials in Table 8.15 should be dissolved in water of specific conductivity not greater than 5 micromhos. The tartrate, phthalate, and phosphates can be dried for 2 h at 100°C before use. Potassium tetroxalate and calcium hydroxide need not be dried. Fresh-looking crystals of borax should be used. Before use, excess solid potassium hydrogen tartrate and calcium hydroxide must be removed. Buffer solutions pH 6 or above should be stored in plastic containers and should be protected from carbon dioxide with soda-lime traps. The solutions should be replaced within 2 to 3 weeks, or sooner if formation of mold is noticed. A crystal of thymol may be added as a preservative.

8.3.2 Standards for pH Measurement of Blood and Biological Media

Blood is a well-buffered medium. In addition to the NBS phosphate standard of 0.025 *M* (pH<sub>s</sub> = 6.480 at 38°C), another reference solution containing the same salts, but in the molal ratio 1 : 4, has an ionic strength of 0.13. It is prepared by dissolving 1.360 g of KH<sub>2</sub>PO<sub>4</sub> and 5.677 g of Na<sub>2</sub>HPO<sub>4</sub> (air weights) in carbon dioxide-free water to make 1 liter of solution. The pH<sub>s</sub> is 7.416 ± 0.004 at 37.5 and 38°C.

The compositions and pH<sub>s</sub> values of *tris*(hydroxymethyl)aminomethane, covering the pH range 7.0 to 8.9, are listed in Table 8.16.

**TABLE 8.16** Composition and pH Values of Buffer Solutions

Values based on the conventional activity pH scale as defined by the National Bureau of Standards (U.S.) and pertain to a temperature of 25°C [Ref: Bower and Bates, *J. Research Natl. Bur. Standards (U.S.)*, **55**:197 (1955) and Bates and Bower, *Anal. Chem.*, **28**:1322 (1956)]. Buffer value is denoted by column headed  $\beta$ .

| 25 ml 0.2M KCl +<br>x ml 0.2M HCl,<br>Diluted to 100 ml                                                                 |      |         | 50 ml 0.1M KH Phthalate<br>+ x ml 0.1M HCl,<br>Diluted to 100 ml                                                                                      |      |         | 50 ml 0.1M KH Phthalate<br>+ x ml 0.1M NaOH,<br>Diluted to 100 ml                                                                           |      |         |
|-------------------------------------------------------------------------------------------------------------------------|------|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------|------|---------|---------------------------------------------------------------------------------------------------------------------------------------------|------|---------|
| pH                                                                                                                      | x    | $\beta$ | pH                                                                                                                                                    | x    | $\beta$ | pH                                                                                                                                          | x    | $\beta$ |
| 1.00                                                                                                                    | 67.0 | 0.31    | 2.20                                                                                                                                                  | 49.5 |         | 4.20                                                                                                                                        | 3.0  | 0.017   |
| 1.20                                                                                                                    | 42.5 | 0.34    | 2.40                                                                                                                                                  | 42.2 | 0.036   | 4.40                                                                                                                                        | 6.6  | 0.020   |
| 1.40                                                                                                                    | 26.6 | 0.19    | 2.60                                                                                                                                                  | 35.4 | 0.033   | 4.60                                                                                                                                        | 11.1 | 0.025   |
| 1.60                                                                                                                    | 16.2 | 0.077   | 2.80                                                                                                                                                  | 28.9 | 0.032   | 4.80                                                                                                                                        | 16.5 | 0.029   |
| 1.80                                                                                                                    | 10.2 | 0.049   | 3.00                                                                                                                                                  | 22.3 | 0.030   | 5.00                                                                                                                                        | 22.6 | 0.031   |
| 2.00                                                                                                                    | 6.5  | 0.030   | 3.20                                                                                                                                                  | 15.7 | 0.026   | 5.20                                                                                                                                        | 28.8 | 0.030   |
| 2.20                                                                                                                    | 3.9  | 0.022   | 3.40                                                                                                                                                  | 10.4 | 0.023   | 5.40                                                                                                                                        | 34.1 | 0.025   |
|                                                                                                                         |      |         | 3.60                                                                                                                                                  | 6.3  | 0.018   | 5.60                                                                                                                                        | 38.8 | 0.020   |
|                                                                                                                         |      |         | 3.80                                                                                                                                                  | 2.9  | 0.015   | 5.80                                                                                                                                        | 42.3 | 0.015   |
| 50 ml 0.1M $\text{KH}_2\text{PO}_4$<br>+ x ml 0.1M NaOH,<br>Diluted to 100 ml                                           |      |         | 50 ml 0.1M Tris(hydroxy-<br>methyl)aminomethane +<br>x ml 0.1M HCl,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.028$<br>$I = 0.001x$ |      |         | 50 ml of a Mixture<br>0.1M with Respect to<br>Both KCl and $\text{H}_3\text{BO}_3$<br>+ x ml 0.1M NaOH,<br>Diluted to 100 ml                |      |         |
| pH                                                                                                                      | x    | $\beta$ | pH                                                                                                                                                    | x    | $\beta$ | pH                                                                                                                                          | x    | $\beta$ |
| 5.80                                                                                                                    | 3.6  |         | 7.00                                                                                                                                                  | 46.6 |         | 8.00                                                                                                                                        | 3.9  |         |
| 6.00                                                                                                                    | 5.6  | 0.010   | 7.20                                                                                                                                                  | 44.7 | 0.012   | 8.20                                                                                                                                        | 6.0  | 0.011   |
| 6.20                                                                                                                    | 8.1  | 0.015   | 7.40                                                                                                                                                  | 42.0 | 0.015   | 8.40                                                                                                                                        | 8.6  | 0.015   |
| 6.40                                                                                                                    | 11.6 | 0.021   | 7.60                                                                                                                                                  | 38.5 | 0.018   | 8.60                                                                                                                                        | 11.8 | 0.018   |
| 6.60                                                                                                                    | 16.4 | 0.027   | 7.80                                                                                                                                                  | 34.5 | 0.023   | 8.80                                                                                                                                        | 15.8 | 0.022   |
| 6.80                                                                                                                    | 22.4 | 0.033   | 8.00                                                                                                                                                  | 29.2 | 0.029   | 9.00                                                                                                                                        | 20.8 | 0.027   |
| 7.00                                                                                                                    | 29.1 | 0.031   | 8.20                                                                                                                                                  | 22.9 | 0.031   | 9.20                                                                                                                                        | 26.4 | 0.029   |
| 7.20                                                                                                                    | 34.7 | 0.025   | 8.40                                                                                                                                                  | 17.2 | 0.026   | 9.40                                                                                                                                        | 32.1 | 0.027   |
| 7.40                                                                                                                    | 39.1 | 0.020   | 8.60                                                                                                                                                  | 12.4 | 0.022   | 9.60                                                                                                                                        | 36.9 | 0.022   |
| 7.60                                                                                                                    | 42.4 | 0.013   | 8.80                                                                                                                                                  | 8.5  | 0.016   | 9.80                                                                                                                                        | 40.6 | 0.016   |
| 7.80                                                                                                                    | 44.5 | 0.009   | 9.00                                                                                                                                                  | 5.7  |         | 10.00                                                                                                                                       | 43.7 | 0.014   |
| 8.00                                                                                                                    | 46.1 |         |                                                                                                                                                       |      |         | 10.20                                                                                                                                       | 46.2 |         |
| 50 ml 0.025M Borax<br>+ x ml 0.1M HCl,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.008$<br>$I = 0.025$ |      |         | 50 ml 0.025M Borax<br>+ x ml 0.1M NaOH,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.008$<br>$I = 0.001(25 + x)$                      |      |         | 50 ml 0.05M $\text{NaHCO}_3$<br>+ x ml 0.1M NaOH,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.009$<br>$I = 0.001(25 + 2x)$ |      |         |
| pH                                                                                                                      | x    | $\beta$ | pH                                                                                                                                                    | x    | $\beta$ | pH                                                                                                                                          | x    | $\beta$ |
| 8.00                                                                                                                    | 20.5 |         | 9.20                                                                                                                                                  | 0.9  |         | 9.60                                                                                                                                        | 5.0  |         |
| 8.20                                                                                                                    | 19.7 | 0.010   | 9.40                                                                                                                                                  | 3.6  | 0.026   | 9.80                                                                                                                                        | 6.2  | 0.014   |
| 8.40                                                                                                                    | 16.6 | 0.012   | 9.60                                                                                                                                                  | 11.1 | 0.022   | 10.00                                                                                                                                       | 10.7 | 0.016   |
| 8.60                                                                                                                    | 13.5 | 0.018   | 9.80                                                                                                                                                  | 15.0 | 0.018   | 10.20                                                                                                                                       | 13.8 | 0.015   |
| 8.80                                                                                                                    | 9.4  | 0.023   | 10.00                                                                                                                                                 | 18.3 | 0.014   | 10.40                                                                                                                                       | 16.5 | 0.013   |

TABLE 8.16 Composition and pH Values of Buffer Solutions (Continued)

|                                                                                                                                                                                    |          |         |                                                                                                                                                         |                                                                                                                                                      |          |                                                                                                                                                                      |          |         |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|---------|
| 50 ml 0.025 <i>M</i> Borax<br>+ <i>x</i> ml 0.1 <i>M</i> HCl,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.008$<br>$I = 0.025$                                     |          |         | 50 ml 0.025 <i>M</i> Borax<br>+ <i>x</i> ml 0.1 <i>M</i> NaOH,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.008$<br>$I = 0.001(25 + x)$ |                                                                                                                                                      |          | 50 ml 0.05 <i>M</i> NaHCO <sub>3</sub><br>+ <i>x</i> ml 0.1 <i>M</i> NaOH,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.009$<br>$I = 0.001(25 + 2x)$ |          |         |
| pH                                                                                                                                                                                 | <i>x</i> | $\beta$ | pH                                                                                                                                                      | <i>x</i>                                                                                                                                             | $\beta$  | pH                                                                                                                                                                   | <i>x</i> | $\beta$ |
| 9.00                                                                                                                                                                               | 4.6      | 0.026   | 10.20                                                                                                                                                   | 20.5                                                                                                                                                 | 0.009    | 10.60                                                                                                                                                                | 19.1     | 0.012   |
| 9.10                                                                                                                                                                               | 2.0      |         | 10.40                                                                                                                                                   | 22.1                                                                                                                                                 | 0.007    | 10.80                                                                                                                                                                | 21.2     | 0.009   |
|                                                                                                                                                                                    |          |         | 10.60                                                                                                                                                   | 23.3                                                                                                                                                 | 0.005    | 11.00                                                                                                                                                                | 22.7     |         |
| 50 ml 0.05 <i>M</i> Na <sub>2</sub> HPO <sub>4</sub><br>+ <i>x</i> ml 0.1 <i>M</i> NaOH,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.025$<br>$I = 0.001(77 + 2x)$ |          |         |                                                                                                                                                         | 25 ml 0.2 <i>M</i> KCl +<br><i>x</i> ml 0.2 <i>M</i> NaOH,<br>Diluted to 100 ml<br>$\Delta\text{pH}/\Delta t \approx -0.033$<br>$I = 0.001(50 + 2x)$ |          |                                                                                                                                                                      |          |         |
| pH                                                                                                                                                                                 | <i>x</i> | $\beta$ | pH                                                                                                                                                      |                                                                                                                                                      | <i>x</i> | $\beta$                                                                                                                                                              |          |         |
| 11.00                                                                                                                                                                              | 4.1      | 0.009   | 12.00                                                                                                                                                   |                                                                                                                                                      | 6.0      | 0.028                                                                                                                                                                |          |         |
| 11.20                                                                                                                                                                              | 6.3      | 0.012   | 12.20                                                                                                                                                   |                                                                                                                                                      | 10.2     | 0.048                                                                                                                                                                |          |         |
| 11.40                                                                                                                                                                              | 9.1      | 0.017   | 12.40                                                                                                                                                   |                                                                                                                                                      | 16.2     | 0.076                                                                                                                                                                |          |         |
| 11.60                                                                                                                                                                              | 13.5     | 0.026   | 12.60                                                                                                                                                   |                                                                                                                                                      | 25.6     | 0.12                                                                                                                                                                 |          |         |
| 11.80                                                                                                                                                                              | 19.4     | 0.034   | 12.80                                                                                                                                                   |                                                                                                                                                      | 41.2     | 0.21                                                                                                                                                                 |          |         |
| 11.90                                                                                                                                                                              | 23.0     | 0.037   | 13.00                                                                                                                                                   |                                                                                                                                                      | 66.0     | 0.30                                                                                                                                                                 |          |         |

The phosphate-succinate system gives the values of pH<sub>s</sub> shown below:

|                                             |   |                                                                           |                 |                                |
|---------------------------------------------|---|---------------------------------------------------------------------------|-----------------|--------------------------------|
| Molality<br>KH <sub>2</sub> PO <sub>4</sub> | = | Molality<br>Na <sub>2</sub> HC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> | pH <sub>s</sub> | $\Delta(\text{pH}_s/\Delta t)$ |
| 0.005                                       |   |                                                                           | 6.251           | − 0.000 86 deg <sup>−1</sup>   |
| 0.010                                       |   |                                                                           | 6.197           | − 0.000 71                     |
| 0.015                                       |   |                                                                           | 6.162           |                                |
| 0.020                                       |   |                                                                           | 6.131           |                                |
| 0.025                                       |   |                                                                           | 6.109           | − 0.000 4                      |

**TABLE 8.17** Standard Reference Values  $\text{pH}_s^*$  for the Measurement of Acidity in 50 Weight Percent Methanol-Water

| Temperature,<br>°C | 0.02 <i>m</i> HOAc,<br>0.02 <i>m</i> NaOAc,<br>0.02 <i>m</i> NaCl | 0.02 <i>m</i> NaHSuc,<br>0.02 <i>m</i> NaCl | 0.02 <i>m</i> $\text{KH}_2\text{PO}_4$ ,<br>0.02 <i>m</i> $\text{Na}_2\text{HPO}_4$ ,<br>0.02 <i>m</i> NaCl |
|--------------------|-------------------------------------------------------------------|---------------------------------------------|-------------------------------------------------------------------------------------------------------------|
| 10                 | 5.560                                                             | 5.806                                       | 7.937                                                                                                       |
| 15                 | 5.549                                                             | 5.786                                       | 7.916                                                                                                       |
| 20                 | 5.543                                                             | 5.770                                       | 7.898                                                                                                       |
| 25                 | 5.540                                                             | 5.757                                       | 7.884                                                                                                       |
| 30                 | 5.540                                                             | 5.748                                       | 7.872                                                                                                       |
| 35                 | 5.543                                                             | 5.743                                       | 7.863                                                                                                       |
| 40                 | 5.550                                                             | 5.741                                       | 7.858                                                                                                       |

OAc = acetate

Suc = succinate

**Reference:** R. G. Bates, *Anal Chem.*, **40**(6):35A (1968).**TABLE 8.18**  $\text{pH}^*$  Values for Buffer Solutions in Alcohol-Water Solvents at 25°C*Liquid-junction potential not included.*

| Solvent<br>Composition<br>(weight per<br>cent alcohol) | 0.01 <i>M</i> $\text{H}_2\text{C}_2\text{O}_4$ ,<br>0.01 <i>M</i> $\text{NH}_4\text{HC}_2\text{O}_4$ | 0.01 <i>M</i> $\text{H}_2\text{Suc}$ ,<br>0.01 <i>M</i> $\text{LiHSuc}$ | 0.01 <i>M</i> $\text{HSal}$ ,<br>0.01 <i>M</i> $\text{NaSal}$ |
|--------------------------------------------------------|------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------|---------------------------------------------------------------|
|                                                        | Methanol-Water Solvents                                                                              |                                                                         |                                                               |
| 0                                                      | 2.15                                                                                                 | 4.12                                                                    |                                                               |
| 10                                                     | 2.19                                                                                                 | 4.30                                                                    |                                                               |
| 20                                                     | 2.25                                                                                                 | 4.48                                                                    |                                                               |
| 30                                                     | 2.30                                                                                                 | 4.67                                                                    |                                                               |
| 40                                                     | 2.38                                                                                                 | 4.87                                                                    |                                                               |
| 50                                                     | 2.47                                                                                                 | 5.07                                                                    |                                                               |
| 60                                                     | 2.58                                                                                                 | 5.30                                                                    |                                                               |
| 70                                                     | 2.76                                                                                                 | 5.57                                                                    |                                                               |
| 80                                                     | 3.13                                                                                                 | 6.01                                                                    |                                                               |
| 90                                                     | 3.73                                                                                                 | 6.73                                                                    |                                                               |
| 92                                                     | 3.90                                                                                                 | 6.92                                                                    |                                                               |
| 94                                                     | 4.10                                                                                                 | 7.13                                                                    |                                                               |
| 96                                                     | 4.39                                                                                                 | 7.43                                                                    |                                                               |
| 98                                                     | 4.84                                                                                                 | 7.89                                                                    |                                                               |
| 99                                                     | 5.20                                                                                                 | 8.23                                                                    |                                                               |
| 100                                                    | 5.79                                                                                                 | 8.75                                                                    | 7.53                                                          |
|                                                        | Ethanol-Water Solvents                                                                               |                                                                         |                                                               |
| 0                                                      | 2.15                                                                                                 | 4.12                                                                    |                                                               |
| 30                                                     | 2.32                                                                                                 | 4.70                                                                    |                                                               |
| 50                                                     | 2.51                                                                                                 | 5.07                                                                    |                                                               |
| 71.9                                                   | 2.98                                                                                                 | 5.71                                                                    |                                                               |
| 100                                                    |                                                                                                      |                                                                         | 8.32                                                          |

Suc = succinate

Sal = salicylate

8.3.3 Buffer Solutions Other Than Standards

The range of the buffering effect of a single weak acid group is approximately one pH unit on either side of the  $pK_a$ . The ranges of some useful buffer systems are collected in Table 8.19. After all the components have been brought together, the pH of the resulting solution should be determined at the temperature to be employed with reference to standard reference solutions. Buffer components should be compatible with other components in the system under study; this is particularly significant for buffers employed in biological studies. Check tables of formation constants to ascertain whether metal-binding character exists.

TABLE 8.19 pH Values of Biological and Other Buffers for Control Purposes

| Materials                                                                        | Acronym             | $pK_a$      | pH range |
|----------------------------------------------------------------------------------|---------------------|-------------|----------|
| <i>p</i> -Toluenesulfonate and <i>p</i> -toluenesulfonic acid                    |                     | 1.7         | 1.1–3.3  |
| Glycine and HCl                                                                  |                     | 2.35        | 1.0–3.7  |
| Citrate and HCl                                                                  |                     | 3.13        | 1.3–4.7  |
| Formate and HCl                                                                  |                     | 3.71        | 2.8–4.6  |
| Succinate and borax                                                              |                     | 4.21, 5.64  | 3.0–5.8  |
| Phenyl acetate and HCl                                                           |                     | 4.31        | 3.5–5.0  |
| Acetate and acetic acid                                                          |                     | 4.76        | 3.7–5.6  |
| Succinate and succinic acid                                                      |                     | 4.21, 5.64  | 4.8–6.3  |
| 2-( <i>N</i> -Morpholino)ethanesulfonic acid                                     | MES                 | 6.1         | 5.5–6.7  |
| Bis(2-hydroxyethyl)iminotris(hydroxymethyl)methane                               | BIS-TRIS            | 6.5         | 5.8–7.2  |
| KH <sub>2</sub> PO <sub>4</sub> and borax                                        |                     | 2.2, 7.2; 9 | 5.8–9.2  |
| <i>N</i> -(2-Acetamido)-2-iminodiacetic acid                                     | ADA                 | 6.6         | 6.0–7.2  |
| 2-[(2-Amino-2-oxoethyl)amino]ethanesulfonic acid                                 | ACES                | 6.8         | 6.1–7.5  |
| Piperazine- <i>N,N'</i> -bis(2-ethanesulfonic acid)                              | PIPES               | 6.8         | 6.1–7.5  |
| 3-( <i>N</i> -Morpholino)-2-hydroxypropanesulfonic acid                          | MOPSO               | 6.9         | 6.2–7.6  |
| 1,3-Bis[tris(hydroxymethyl)methylamino]propane                                   | BIS-TRIS<br>PROPANE | 6.8, 9.0    | 6.3–9.5  |
| KH <sub>2</sub> PO <sub>4</sub> and Na <sub>2</sub> HPO <sub>4</sub>             |                     | 7.2         | 6.1–7.5  |
| <i>N,N</i> -Bis(2-hydroxyethyl)-2-aminoethanesulfonic acid                       | BES                 | 7.1         | 6.4–7.8  |
| 3-( <i>N</i> -Morpholino)propanesulfonic acid                                    | MOPS                | 7.2         | 6.5–7.9  |
| <i>N</i> -(2-Hydroxyethyl)piperazine- <i>N'</i> -(2-ethanesulfonic acid)         | HEPES               | 7.5         | 6.8–8.2  |
| <i>N</i> -Tris(hydroxymethyl)methyl-2-aminoethanesulfonic acid                   | TES                 | 7.5         | 6.8–8.2  |
| 3-[ <i>N,N</i> -Bis(2-hydroxyethyl)amino]-2-hydroxypropanesulfonic acid          | DIPSO               | 7.6         | 7.0–8.2  |
| 3-[ <i>N</i> -tris(hydroxymethyl)methylamino]-2-hydroxypropanesulfonic acid      | TAPSO               | 7.6         | 7.0–8.2  |
| 5,5-Diethylbarbiturate (veronal) and HCl                                         |                     | 8.0         | 7.0–8.5  |
| Tris(hydroxymethyl)aminoethane                                                   | TRIZMA              | 8.1         | 7.0–9.1  |
| <i>N</i> -(2-hydroxyethyl)piperazine- <i>N'</i> -(2-hydroxypropanesulfonic acid) | HEPPSO              | 7.8         | 7.1–8.5  |
| Piperazine- <i>N,N'</i> -bis(2-hydroxypropanesulfonic acid)                      | POPSO               | 7.8         | 7.2–8.5  |
| Triethanolamine                                                                  | TEA                 | 7.8         | 6.9–8.5  |
| <i>N</i> -Tris(hydroxymethyl)methylglycine                                       | TRICINE             | 8.1         | 7.4–8.8  |
| Borax and HCl                                                                    |                     |             | 7.6–8.9  |
| <i>N,N</i> -Bis(2-hydroxyethyl)glycine                                           | BICINE              | 8.3         | 7.6–9.0  |
| <i>N</i> -Tris(hydroxymethyl)methyl-3-aminopropanesulfonic acid                  | TAPS                | 8.4         | 7.7–9.1  |
| 3-[(1,1-Dimethyl-2-hydroxyethyl)-2-hydroxypropanesulfonic acid                   | AMPSO               | 9.0         | 8.3–9.7  |
| Ammonia (aqueous) and NH <sub>4</sub> Cl                                         |                     | 9.2         | 8.3–9.2  |
| 2-( <i>N</i> -Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid                  | CHES                | 9.3         | 8.6–10.0 |

**TABLE 8.19** pH Values of Biological and Other Buffers for Control Purposes (*Continued*)

| Materials                                            |  |  | Acronym | pK <sub>a</sub> | pH range  |
|------------------------------------------------------|--|--|---------|-----------------|-----------|
| Glycine and NaOH                                     |  |  |         | 9.7             | 8.2–10.1  |
| Ethanolamine (2-aminoethanol) and HCl                |  |  |         | 9.5             | 8.6–10.4  |
| 3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid |  |  | CAPSO   | 9.6             | 8.9–10.3  |
| 2-Amino-2-methyl-1-propanol                          |  |  | AMP     | 9.7             | 9.0–10.5  |
| Carbonate and hydrogen carbonate                     |  |  |         | 10.3            | 9.2–11.0  |
| Borax and NaOH                                       |  |  |         |                 | 9.4–11.1  |
| 3-(Cyclohexylamino)-1-propanesulfonic acid           |  |  | CAPS    | 10.4            | 9.7–11.1  |
| Na <sub>2</sub> HPO <sub>4</sub> and NaOH            |  |  |         | 11.9            | 11.0–12.0 |

|                                                                                                          |           |                 |                                                                                                                                                                                                      |                                      |           |      |                                      |           |
|----------------------------------------------------------------------------------------------------------|-----------|-----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------|-----------|------|--------------------------------------|-----------|
| x mL of 0.2M Sodium Acetate (27.199 g NaOAc · 3H <sub>2</sub> O per liter) plus y mL of 0.2M Acetic Acid |           |                 | x mL of 0.1M KH <sub>2</sub> PO <sub>4</sub> (13.617 g · L <sup>-1</sup> ) plus y mL of 0.05M Borax Solution (19.404 g Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> · 10H <sub>2</sub> O per Liter) |                                      |           |      |                                      |           |
| pH                                                                                                       | NaOAc, mL | Acetic Acid, mL | pH                                                                                                                                                                                                   | KH <sub>2</sub> PO <sub>4</sub> , mL | Borax, mL | pH   | KH <sub>2</sub> PO <sub>4</sub> , mL | Borax, mL |
| 3.60                                                                                                     | 7.5       | 92.5            | 5.80                                                                                                                                                                                                 | 92.1                                 | 7.9       | 7.60 | 51.7                                 | 48.3      |
| 3.80                                                                                                     | 12.0      | 88.0            | 6.00                                                                                                                                                                                                 | 87.7                                 | 12.3      | 7.80 | 49.2                                 | 50.8      |
| 4.00                                                                                                     | 18.0      | 82.0            | 6.200                                                                                                                                                                                                | 83.0                                 | 17.0      | 8.00 | 46.5                                 | 53.5      |
| 4.20                                                                                                     | 26.5      | 73.5            | 6.40                                                                                                                                                                                                 | 77.8                                 | 22.2      | 8.20 | 43.0                                 | 57.0      |
| 4.40                                                                                                     | 37.0      | 63.0            | 6.60                                                                                                                                                                                                 | 72.2                                 | 27.8      | 8.40 | 38.7                                 | 61.3      |
| 4.60                                                                                                     | 49.0      | 51.0            | 6.80                                                                                                                                                                                                 | 66.7                                 | 33.3      | 8.60 | 34.0                                 | 66.0      |
| 4.80                                                                                                     | 60.0      | 40.0            | 7.00                                                                                                                                                                                                 | 62.3                                 | 37.7      | 8.80 | 27.6                                 | 72.4      |
| 5.00                                                                                                     | 70.5      | 29.5            | 7.20                                                                                                                                                                                                 | 58.1                                 | 41.9      | 9.00 | 17.5                                 | 82.5      |
| 5.20                                                                                                     | 79.0      | 21.0            | 7.40                                                                                                                                                                                                 | 55.0                                 | 45.0      | 9.20 | 5.0                                  | 95.0      |
| 5.40                                                                                                     | 85.5      | 14.5            |                                                                                                                                                                                                      |                                      |           |      |                                      |           |
| 5.60                                                                                                     | 90.5      | 9.5             |                                                                                                                                                                                                      |                                      |           |      |                                      |           |

|                                                                                |             |         |                                                                                                                  |                         |                        |                                                                                                         |             |          |
|--------------------------------------------------------------------------------|-------------|---------|------------------------------------------------------------------------------------------------------------------|-------------------------|------------------------|---------------------------------------------------------------------------------------------------------|-------------|----------|
| x mL of Veronal (20.6 g Na Diethylbarbiturate per Liter) plus y mL of 0.1M HCl |             |         | x mL of 0.2M Aqueous NH <sub>3</sub> Solution plus y mL of 0.2M NH <sub>4</sub> Cl (10.699 g · L <sup>-1</sup> ) |                         |                        | x mL of 0.1M Citrate (21.0 g Citric Acid Monohydrate + 200 mL 1M NaOH per Liter) plus y mL of 0.1M NaOH |             |          |
| pH                                                                             | Veronal, mL | HCl, mL | pH                                                                                                               | Aq NH <sub>3</sub> , mL | NH <sub>4</sub> Cl, mL | pH                                                                                                      | Citrate, mL | NaOH, mL |
| 7.00                                                                           | 53.6        | 46.4    | 8.00                                                                                                             | 5.5                     | 94.5                   | 5.10                                                                                                    | 90.0        | 10.0     |
| 7.20                                                                           | 55.4        | 44.6    | 8.20                                                                                                             | 8.5                     | 91.5                   | 5.30                                                                                                    | 80.0        | 20.0     |
| 7.40                                                                           | 58.1        | 41.9    | 8.40                                                                                                             | 12.5                    | 87.5                   | 5.50                                                                                                    | 71.0        | 29.0     |
| 7.60                                                                           | 61.5        | 38.5    | 8.60                                                                                                             | 18.5                    | 81.5                   | 5.70                                                                                                    | 67.0        | 33.0     |
| 7.80                                                                           | 66.2        | 33.8    | 8.80                                                                                                             | 26.0                    | 74.0                   | 5.90                                                                                                    | 62.0        | 38.0     |
| 8.00                                                                           | 71.6        | 28.4    | 9.00                                                                                                             | 36.0                    | 64.0                   |                                                                                                         |             |          |
| 8.20                                                                           | 76.9        | 23.1    | 9.25                                                                                                             | 50.0                    | 50.0                   |                                                                                                         |             |          |
| 8.40                                                                           | 82.3        | 17.7    | 9.40                                                                                                             | 58.5                    | 41.5                   |                                                                                                         |             |          |
| 8.60                                                                           | 87.1        | 12.9    | 9.60                                                                                                             | 69.0                    | 31.0                   |                                                                                                         |             |          |
| 8.80                                                                           | 90.8        | 9.2     | 9.80                                                                                                             | 78.0                    | 22.0                   |                                                                                                         |             |          |
| 9.00                                                                           | 93.6        | 6.4     | 10.00                                                                                                            | 85.0                    | 15.0                   |                                                                                                         |             |          |



**TABLE 8.19** pH Values of Biological and Other Buffers for Control Purposes (*Continued*)

| x mL of 0.2M NaOH Added to 100 mL of Stock Solution<br>(0.04M Acetic Acid, 0.04M H <sub>3</sub> PO <sub>4</sub> , and 0.04M Boric Acid)                        |                                          |                    |                                                                                                                   |                                          |                    |                                                                                                                                                                                      |                                          |                    |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------|--------------------|-------------------------------------------------------------------------------------------------------------------|------------------------------------------|--------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------|--------------------|
| pH                                                                                                                                                             | NaOH, mL                                 |                    | pH                                                                                                                | NaOH, mL                                 |                    | pH                                                                                                                                                                                   | NaOH, mL                                 |                    |
| 1.81                                                                                                                                                           | 0.0                                      |                    | 4.10                                                                                                              | 25.0                                     |                    | 6.80                                                                                                                                                                                 | 50.0                                     |                    |
| 1.89                                                                                                                                                           | 2.5                                      |                    | 4.35                                                                                                              | 27.5                                     |                    | 7.00                                                                                                                                                                                 | 52.5                                     |                    |
| 1.98                                                                                                                                                           | 5.0                                      |                    | 4.56                                                                                                              | 30.0                                     |                    | 7.24                                                                                                                                                                                 | 55.0                                     |                    |
| 2.09                                                                                                                                                           | 7.5                                      |                    | 4.78                                                                                                              | 32.5                                     |                    | 7.54                                                                                                                                                                                 | 57.5                                     |                    |
| 2.21                                                                                                                                                           | 10.0                                     |                    | 5.02                                                                                                              | 35.0                                     |                    | 7.96                                                                                                                                                                                 | 60.0                                     |                    |
| 2.36                                                                                                                                                           | 12.5                                     |                    | 5.33                                                                                                              | 37.5                                     |                    | 8.36                                                                                                                                                                                 | 62.5                                     |                    |
| 2.56                                                                                                                                                           | 15.0                                     |                    | 5.72                                                                                                              | 40.0                                     |                    | 8.69                                                                                                                                                                                 | 65.0                                     |                    |
| 2.87                                                                                                                                                           | 17.5                                     |                    | 6.09                                                                                                              | 42.5                                     |                    | 8.95                                                                                                                                                                                 | 67.5                                     |                    |
| 3.29                                                                                                                                                           | 20.0                                     |                    | 6.37                                                                                                              | 45.0                                     |                    | 9.15                                                                                                                                                                                 | 70.0                                     |                    |
| 3.78                                                                                                                                                           | 22.5                                     |                    | 6.59                                                                                                              | 47.5                                     |                    | 9.37                                                                                                                                                                                 | 72.5                                     |                    |
|                                                                                                                                                                |                                          |                    |                                                                                                                   |                                          |                    |                                                                                                                                                                                      |                                          |                    |
| x mL of 0.1M HCl plus<br>y mL of 0.1M Glycine<br>(7.505 g Glycine +<br>5.85 g NaCl per Liter)                                                                  |                                          |                    | x mL of 0.1M HCl plus y mL<br>of 0.1M Citrate (21.008 g<br>Citric Acid Monohydrate +<br>200 ml 1M NaOH per Liter) |                                          |                    | x mL of 0.05M Succinic Acid<br>(5.90 g · L <sup>-1</sup> ) plus y mL of<br>Borax Solution (19.404 g<br>Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> · 10H <sub>2</sub> O per Liter) |                                          |                    |
| pH                                                                                                                                                             | HCl,<br>mL                               | Glycine,<br>mL     | pH                                                                                                                | HCl,<br>mL                               | Citrate,<br>mL     | pH                                                                                                                                                                                   | Succinic<br>Acid, mL                     | Borax,<br>mL       |
| 1.20                                                                                                                                                           | 84.0                                     | 16.0               | 3.50                                                                                                              | 52.8                                     | 47.2               | 3.60                                                                                                                                                                                 | 90.5                                     | 9.5                |
| 1.40                                                                                                                                                           | 71.0                                     | 29.0               | 3.60                                                                                                              | 51.3                                     | 48.7               | 3.80                                                                                                                                                                                 | 86.3                                     | 13.7               |
| 1.60                                                                                                                                                           | 61.8                                     | 38.2               | 3.80                                                                                                              | 48.6                                     | 51.4               | 4.00                                                                                                                                                                                 | 82.2                                     | 17.8               |
| 1.80                                                                                                                                                           | 55.2                                     | 44.8               | 4.00                                                                                                              | 43.8                                     | 56.2               | 4.20                                                                                                                                                                                 | 77.8                                     | 22.2               |
| 2.00                                                                                                                                                           | 49.1                                     | 50.9               | 4.20                                                                                                              | 38.6                                     | 61.4               | 4.40                                                                                                                                                                                 | 73.8                                     | 26.2               |
| 2.20                                                                                                                                                           | 42.7                                     | 57.3               | 4.40                                                                                                              | 34.6                                     | 65.4               | 4.60                                                                                                                                                                                 | 70.0                                     | 30.0               |
| 2.40                                                                                                                                                           | 36.5                                     | 63.5               | 4.60                                                                                                              | 24.3                                     | 75.7               | 4.80                                                                                                                                                                                 | 66.5                                     | 33.5               |
| 2.60                                                                                                                                                           | 30.3                                     | 69.7               | 4.80                                                                                                              | 11.0                                     | 89.0               | 5.00                                                                                                                                                                                 | 63.2                                     | 36.8               |
| 2.80                                                                                                                                                           | 24.0                                     | 76.0               |                                                                                                                   |                                          |                    | 5.20                                                                                                                                                                                 | 60.5                                     | 39.5               |
| 3.00                                                                                                                                                           | 17.8                                     | 82.2               |                                                                                                                   |                                          |                    | 5.40                                                                                                                                                                                 | 57.9                                     | 42.1               |
| 3.30                                                                                                                                                           | 10.8                                     | 89.2               |                                                                                                                   |                                          |                    | 5.60                                                                                                                                                                                 | 55.7                                     | 44.3               |
| 3.60                                                                                                                                                           | 6.0                                      | 94.0               |                                                                                                                   |                                          |                    | 5.80                                                                                                                                                                                 | 54.0                                     | 46.0               |
|                                                                                                                                                                |                                          |                    |                                                                                                                   |                                          |                    |                                                                                                                                                                                      |                                          |                    |
| x mL of 0.2M Na <sub>2</sub> HPO <sub>4</sub> · 2H <sub>2</sub> O (35.599 g · L <sup>-1</sup> ) plus<br>y mL of 0.1M Citric Acid (19.213 g · L <sup>-1</sup> ) |                                          |                    |                                                                                                                   |                                          |                    |                                                                                                                                                                                      |                                          |                    |
| pH                                                                                                                                                             | Na <sub>2</sub> HPO <sub>4</sub> ,<br>mL | Citric<br>Acid, mL | pH                                                                                                                | Na <sub>2</sub> HPO <sub>4</sub> ,<br>mL | Citric<br>Acid, mL | pH                                                                                                                                                                                   | Na <sub>2</sub> HPO <sub>4</sub> ,<br>mL | Citric<br>Acid, mL |
| 2.20                                                                                                                                                           | 2.00                                     | 98.00              | 4.20                                                                                                              | 41.40                                    | 58.60              | 6.20                                                                                                                                                                                 | 66.10                                    | 33.90              |
| 2.40                                                                                                                                                           | 6.20                                     | 93.80              | 4.40                                                                                                              | 44.10                                    | 55.90              | 6.40                                                                                                                                                                                 | 69.25                                    | 30.75              |
| 2.60                                                                                                                                                           | 10.90                                    | 89.10              | 4.60                                                                                                              | 46.75                                    | 53.25              | 6.60                                                                                                                                                                                 | 72.75                                    | 27.25              |
| 2.80                                                                                                                                                           | 15.85                                    | 84.15              | 4.80                                                                                                              | 49.30                                    | 50.70              | 6.80                                                                                                                                                                                 | 77.25                                    | 22.75              |
| 3.00                                                                                                                                                           | 20.55                                    | 79.45              | 5.00                                                                                                              | 51.50                                    | 48.50              | 7.00                                                                                                                                                                                 | 82.35                                    | 17.65              |
| 3.20                                                                                                                                                           | 24.70                                    | 75.30              | 5.20                                                                                                              | 53.60                                    | 46.40              | 7.20                                                                                                                                                                                 | 86.95                                    | 13.05              |
| 3.40                                                                                                                                                           | 28.50                                    | 71.50              | 5.40                                                                                                              | 55.75                                    | 44.25              | 7.40                                                                                                                                                                                 | 90.85                                    | 9.15               |
| 3.60                                                                                                                                                           | 32.20                                    | 67.80              | 5.60                                                                                                              | 58.00                                    | 42.00              | 7.60                                                                                                                                                                                 | 93.65                                    | 6.35               |
| 3.80                                                                                                                                                           | 35.50                                    | 64.50              | 5.80                                                                                                              | 60.45                                    | 39.55              | 7.80                                                                                                                                                                                 | 95.75                                    | 4.25               |
| 4.00                                                                                                                                                           | 38.55                                    | 61.45              | 6.00                                                                                                              | 63.15                                    | 36.85              | 8.00                                                                                                                                                                                 | 97.25                                    | 2.75               |

When there are two or more acid groups per molecule, or a mixture is composed of several overlapping acids, the useful range is larger. Universal buffer solutions consist of a mixture of acid groups which overlap such that successive  $pK_a$  values differ by 2 pH units or less. The Prideaux-Ward mixture comprises phosphate, phenyl acetate, and borate plus HCl and covers the range from 2 to 12 pH units. The McIlvaine buffer is a mixture of citric acid and  $\text{Na}_2\text{HPO}_4$  that covers the range from pH 2.2 to 8.0. The Britton-Robinson system consists of acetic acid, phosphoric acid, and boric acid plus NaOH and covers the range from pH 4.0 to 11.5. A mixture composed of  $\text{Na}_2\text{CO}_3$ ,  $\text{NaH}_2\text{PO}_4$ , citric acid, and 2-amino-2-methyl-1,3-propanediol covers the range from pH 2.2 to 11.0.

General directions for the preparation of buffer solutions of varying pH but fixed ionic strength are given by Bates.\* Preparation of McIlvaine buffered solutions at ionic strengths of 0.5 and 1.0 and Britton-Robinson solutions of constant ionic strength have been described by Elving et al.† and Frugoni,‡ respectively.

\* Bates, *Determination of pH, Theory and Practice*, Wiley, New York, 1964, pp. 121–122.

† Elving, Markowitz, and Rosenthal, *Anal. Chem.*, **28**:1179 (1956).

‡ Frugoni, *Gazz. Chim. Ital.*, **87**:L403 (1957).

## 8.4 REFERENCE ELECTRODES

**TABLE 8.20** Potentials of Reference Electrodes in Volts as a Function of Temperature

*Liquid-junction potential included.*

| Temp.,<br>°C | 0.1M KCl<br>Calomel* | 1.0M KCl<br>Calomel* | 3.5M KCl<br>Calomel* | Satd. KCl<br>Calomel* | 1.0M KCl<br>Ag/AgCl† | 1.0M KBr<br>Ag/AgBr‡ | 1.0M KI<br>Ag/AgI§ |
|--------------|----------------------|----------------------|----------------------|-----------------------|----------------------|----------------------|--------------------|
| 0            | 0.3367               | 0.2883               |                      | 0.25918               | 0.23655              | 0.08128              | −0.14637           |
| 5            |                      |                      |                      |                       | 0.23413              | 0.07961              | −0.14719           |
| 10           | 0.3362               | 0.2868               | 0.2556               | 0.25387               | 0.23142              | 0.07773              | −0.14822           |
| 15           | 0.3361               |                      |                      | 0.2511                | 0.22857              | 0.07572              | −0.14942           |
| 20           | 0.3358               | 0.2844               | 0.2520               | 0.24775               | 0.22557              | 0.07349              | −0.15081           |
| 25           | 0.3356               | 0.2830               | 0.2501               | 0.24453               | 0.22234              | 0.07106              | −0.15244           |
| 30           | 0.3354               | 0.2815               | 0.2481               | 0.24118               | 0.21904              | 0.06856              | −0.15405           |
| 35           | 0.3351               |                      |                      | 0.2376                | 0.21565              | 0.06585              | −0.15590           |
| 38           | 0.3350               |                      | 0.2448               | 0.2355                |                      |                      |                    |
| 40           | 0.3345               | 0.2782               | 0.2439               | 0.23449               | 0.21208              | 0.06310              | −0.15788           |
| 45           |                      |                      |                      |                       | 0.20835              | 0.06012              | −0.15998           |
| 50           | 0.3315               | 0.2745               |                      | 0.22737               | 0.20449              | 0.05704              | −0.16219           |
| 55           |                      |                      |                      |                       | 0.20056              |                      |                    |
| 60           | 0.3248               | 0.2702               |                      | 0.2235                | 0.19649              |                      |                    |
| 70           |                      |                      |                      |                       | 0.18782              |                      |                    |
| 80           |                      |                      |                      | 0.2083                | 0.1787               |                      |                    |
| 90           |                      |                      |                      |                       | 0.1695               | 0.0251               |                    |

\* Bates et al., *J. Research Natl. Bur. Standards*, **45**, 418 (1950).

† Bates and Bower, *J. Research Natl. Bur. Standards*, **53**, 283 (1954).

‡ Hetzer, Robinson and Bates, *J. Phys. Chem.*, **66**, 1423 (1962).

§ Hetzer, Robinson and Bates, *J. Phys. Chem.*, **68**, 1929 (1964).

**TABLE 8.20** Potentials of Reference Electrodes in Volts as a Function of Temperature (*Continued*)

| Temp., °C            | 125     | 150     | 175     | 200     | 225     | 250    | 275    |
|----------------------|---------|---------|---------|---------|---------|--------|--------|
| 1.0M KCl<br>Ag/AgCl* | 0.1330  | 0.1032  | 0.0708  | 0.0348  | −0.0051 | −0.054 | −0.090 |
| 1.0M KBr<br>Ag/AgBr† | −0.0048 | −0.0312 | −0.0612 | −0.0951 |         |        |        |

\* Greeley et al., *J. Phys. Chem.*, **64**, 652 (1960).

† Towns et al., *J. Phys. Chem.*, **64**, 1861 (1960).

The values of several additional reference electrodes at 25°C are listed:

|                                                                                  |       |
|----------------------------------------------------------------------------------|-------|
| Ag/AgCl, satd. KCl                                                               | 0.198 |
| Ag/AgCl, 01M KCl                                                                 | 0.288 |
| Hg/HgO, 1.0M NaOH                                                                | 0.140 |
| Hg/HgO, 0.1M NaOH                                                                | 0.165 |
| Hg/Hg <sub>2</sub> SO <sub>4</sub> , satd. K <sub>2</sub> SO <sub>4</sub> (22°C) | 0.658 |
| Hg/Hg <sub>2</sub> SO <sub>4</sub> , satd. KCl                                   | 0.655 |

**TABLE 8.21** Potentials of Reference Electrodes (in Volts) at 25°C for Water–Organic Solvent Mixtures  
*Electrolyte solution of 1M HCl.*

| Solvent,<br>wt % | Methanol,<br>Ag/AgCl | Ethanol,<br>Ag/AgCl | 2-Propanol,<br>Ag/AgCl | Acetone,<br>Ag/AgCl | Dioxane,<br>Ag/AgCl | Ethylene<br>glycol,<br>Ag/AgCl | Methanol,<br>calomel | Dioxane,<br>calomel |
|------------------|----------------------|---------------------|------------------------|---------------------|---------------------|--------------------------------|----------------------|---------------------|
| 5                |                      |                     | 0.2180                 | 0.2190              |                     | 0.2190                         |                      |                     |
| 10               | 0.2153               | 0.2146              | 0.2138                 | 0.2156              |                     | 0.2160                         |                      |                     |
| 20               | 0.2090               | 0.2075              | 0.2063                 | 0.2079              | 0.2031              | 0.2101                         | 0.255                | 0.2501              |
| 30               |                      | 0.2003              |                        |                     |                     | 0.2036                         |                      |                     |
| 40               | 0.1968               | 0.1945              |                        | 0.1859              |                     | 0.1972                         | 0.243                |                     |
| 45               |                      |                     |                        |                     | 0.1635              |                                |                      | 0.2104              |
| 50               |                      | 0.1859              |                        | 0.158               |                     |                                |                      |                     |
| 60               | 0.1818               | 0.173               |                        |                     |                     | 0.1807                         |                      |                     |
| 70               |                      | 0.158               |                        |                     | 0.0659              |                                | 0.216                | 0.1126              |
| 80               | 0.1492               | 0.136               |                        |                     |                     |                                |                      |                     |
| 82               |                      |                     |                        |                     | −0.0614             |                                |                      | −0.0014             |
| 90               | 0.1135               | 0.096               |                        | −0.034              |                     |                                |                      |                     |
| 94.2             | 0.0841               |                     |                        |                     |                     |                                |                      |                     |
| 98               |                      | 0.0215              |                        |                     |                     |                                |                      |                     |
| 99               |                      |                     |                        |                     |                     |                                | 0.103                |                     |
| 100              | −0.0099              | −0.0081             |                        | −0.53               |                     |                                |                      |                     |

### 8.4.1 Electrometric Measurement of pH

The pH value is defined for an aqueous solution in an operational (arbitrary but reproducible) manner according to the Bates-Guggenheim convention:

$$\text{pH}_x = \text{pH}_s + \frac{E_x - E_s}{2.3026RT/F}$$

where  $R$  is the gas constant per mole,  $T$  is the temperature on the absolute scale, and  $F$  is the faraday. The  $\text{pH}_x$  of the unknown medium is calculated from that of an accepted standard ( $\text{pH}_s$ ) and the measured difference in the emf ( $E$ ) of the electrode combination when the standard solution is removed from the cell and replaced by the unknown. The double vertical line marks a liquid junction. Electrodes as fabricated exhibit variations in the reproducibility of the reference electrode, in the liquid-junction potential, and, with glass electrodes, in the asymmetry potential. These differences are all eliminated in the standardizing procedure with standard reference pH buffers. (See R. G. Bates, *Determination of pH, Theory and Practice*, Wiley, New York, 1964.)

|                                          |                                                     |                                                    |                        |
|------------------------------------------|-----------------------------------------------------|----------------------------------------------------|------------------------|
| Electrode reversible<br>to hydrogen ions | Standard reference<br>buffer or unknown<br>solution | Salt bridge<br>(KCl. 3.5 <i>M</i><br>or saturated) | Reference<br>electrode |
|------------------------------------------|-----------------------------------------------------|----------------------------------------------------|------------------------|

An electrometric pH-measurement system consists of (1) pH-responsive electrode, (2) reference electrode, and (3) potential-measuring device—some form of high-impedance electronic voltmeter for glass-electrode combinations and this or a potentiometer arrangement for other pH-responsive electrodes. Electronic pH meters are simply voltmeters with scale divisions in pH units which are equivalent to the values of  $2.3026RT/F$  (in mV) per pH unit. Values of this function at several temperatures are given in Table 8.22. There is no compensation incorporated in the meter for the changes in pH of the test solution as a function of temperature. Reliability of an indicator–reference electrode combination must be ascertained by standardization of the pH meter with one standard buffer and checking the pH response by immersing the combination in a second and different reference buffer.

The temperature compensator on a pH meter varies the instrument definition of a pH unit from 54.20 mV at 0°C to perhaps 66.10 mV at 60°C. This permits one to measure the pH of the sample (and reference buffer standard) at its actual temperature and thus avoid error due to dissociation equilibria and to junction potentials which have significant temperature coefficients.

**TABLE 8.22** Values of  $2.3026RT/F$  at Several Temperatures

*In millivolts.*

| $t$ °C | Value  | $t$ °C | Value  | $t$ °C | Value  | $t$ °C | Value  |
|--------|--------|--------|--------|--------|--------|--------|--------|
| 0      | 54.197 | 25     | 59.157 | 50     | 64.118 | 80     | 70.070 |
| 5      | 55.189 | 30     | 60.149 | 55     | 65.110 | 85     | 71.062 |
| 10     | 56.181 | 35     | 61.141 | 60     | 66.102 | 90     | 72.054 |
| 15     | 57.173 | 38     | 61.737 | 65     | 67.094 | 95     | 73.046 |
| 18     | 57.767 | 40     | 62.133 | 70     | 68.086 | 100    | 74.038 |
| 20     | 58.165 | 45     | 63.126 | 75     | 69.078 |        |        |

Report of the National Academy of Sciences: National Research Council Committee of Fundamental Constants, 1963.

8.5 INDICATORS

TABLE 8.23 Indicators for Aqueous Acid-Base Titrations

This table lists some selected indicators. The pH range or transition interval given in the third column may vary appreciably from one observer to another, and, in addition, it is affected by ionic strength, temperature, and illumination; consequently only approximate values can be given. They should be considered to refer to solutions having low ionic strengths and a temperature of about 25°C. In the fourth column the  $pK_a$  ( $-\log K_a$ ) of the indicator as determined spectrophotometrically is listed. In the fifth column the wavelength of maximum absorption is given first for the acidic and then for the basic form of the indicator, and the same order is followed in giving the colors in the sixth column. The abbreviations used to describe the colors of the two forms of the indicator are as follows:

B, blue                      G, green  
V, violet                    P, purple  
Y, yellow                  R, red  
O, orange                 O-Br, orange-brown  
C, colorless

| Indicator                     | Chemical name                                     | pH range | $pK_a$ | $\lambda_{\max}$ , nm | Color change |
|-------------------------------|---------------------------------------------------|----------|--------|-----------------------|--------------|
| Cresol red<br>(acid range)    | <i>o</i> -Cresolsulfonephthalein                  | 0.2–1.8  |        |                       | R-Y          |
| Cresol purple<br>(acid range) | <i>m</i> -Cresolsulfonephthalein                  | 1.2–2.8  | 1.51   | 533, —                | R-Y          |
| Thymol blue<br>(acid range)   | Thymolsulfonephthalein                            | 1.2–2.8  | 1.65   | 544, 430              | R-Y          |
| Tropeolin OO                  | Diphenylamino- <i>p</i> -benzene sodium sulfonate | 1.3–3.2  | 2.0    | 527, —                | R-Y          |
| 2,6-Dinitrophenol             | 2,6-Dinitrophenol                                 | 2.4–4.0  | 3.69   |                       | C-Y          |
| 2,4-Dinitrophenol             | 2,4-Dinitrophenol                                 | 2.5–4.3  | 3.90   |                       | C-Y          |
| Methyl yellow                 | Dimethylaminoazobenzene                           | 2.9–4.0  | 3.3    | 508, —                | R-Y          |
| Methyl orange                 | Dimethylaminoazobenzene sodium sulfonate          | 3.1–4.4  | 3.40   | 522, 464              | R-O          |
| Bromophenol blue              | Tetrabromophenolsulfonephthalein                  | 3.0–4.6  | 3.85   | 436, 592              | Y-BV         |
| Bromocresol green             | Tetrabromo- <i>m</i> -cresolsulfonephthalein      | 4.0–5.6  | 4.68   | 444, 617              | Y-B          |
| Methyl red                    | <i>o</i> -Carboxybenzeneazo-dimethylaniline       | 4.4–6.2  | 4.95   | 530, 427              | R-Y          |
| Chlorophenol red              | Dichlorophenolsulfonephthalein                    | 5.4–6.8  | 6.0    | —, 573                | Y-R          |
| Bromocresol purple            | Dibromo- <i>o</i> -cresolsulfonephthalein         | 5.2–6.8  | 6.3    | 433, 591              | Y-P          |
| Bromophenol red               | Dibromophenolsulfonephthalein                     | 5.2–6.8  |        | —, 574                | Y-R          |
| <i>p</i> -Nitrophenol         | <i>p</i> -Nitrophenol                             | 5.3–7.6  | 7.15   | 320, 405              | C-Y          |
| Bromothymol blue              | Dibromothymolsulfonephthalein                     | 6.2–7.6  | 7.1    | 433, 617              | Y-B          |
| Neutral red                   | Aminodimethylaminotoluphenazonium chloride        | 6.8–8.0  | 7.4    |                       | R-Y          |
| Phenol red                    | Phenolsulfonephthalein                            | 6.4–8.0  | 7.9    | 433, 558              | Y-R          |
| <i>m</i> -Nitrophenol         | <i>m</i> -Nitrophenol                             | 6.4–8.8  | 8.3    | —, 570                | C-Y          |

**TABLE 8.23** Indicators for Aqueous Acid-Base Titrations (*Continued*)

| Indicator                 | Chemical name                                          | pH range  | $pK_a$ | $\lambda_{\max}$ , nm | Color change |
|---------------------------|--------------------------------------------------------|-----------|--------|-----------------------|--------------|
| Cresol red                | <i>o</i> -Cresolsulfonephthalein                       | 7.2–8.8   | 8.2    | 434, 572              | Y-R          |
| <i>m</i> -Cresol purple   | <i>m</i> -Cresolsulfonephthalein                       | 7.6–9.2   | 8.32   | —, 580                | Y-P          |
| Thymol blue               | Thymolsulfonephthalein                                 | 8.0–9.6   | 8.9    | 430, 596              | Y-B          |
| Phenolphthalein           | Phenolphthalein                                        | 8.0–10.0  | 9.4    | —, 553                | C-R          |
| $\alpha$ -Naphtholbenzein | $\alpha$ -Naphtholbenzein                              | 9.0–11.0  |        |                       | Y-B          |
| Thymolphthalein           | Thymolphthalein                                        | 9.4–10.6  | 10.0   | —, 598                | C-B          |
| Alizarin Yellow R         | 5-( <i>p</i> -Nitrophenylazo)-salicyclic acid, Na salt | 10.0–12.0 | 11.16  |                       | Y-V          |
| Tropeolin O               | <i>p</i> -Sulfobenzenazo-resorcinol                    | 11.0–13.0 |        |                       | Y-O-Br       |
| Nitramine                 | 2,4,6-Trinitrophenyl-methylnitroamine                  | 10.8–13.0 |        |                       | C-O-Br       |

**TABLE 8.24** Mixed Indicators

Mixed indicators give sharp color changes and are especially useful in titrating to a given titration exponent ( $pI$ ).

The information given in this table is from the two-volume work *Volumetric Analysis* by Kolthoff and Stenger, published by Interscience Publishers, Inc., New York, 1942 and 1947, and reproduced with their permission.

| Composition of Indicator Solution                | $pI$ | Color        |             | Notes                                                                        |
|--------------------------------------------------|------|--------------|-------------|------------------------------------------------------------------------------|
|                                                  |      | Acid         | Alkaline    |                                                                              |
| 1 part 0.1% methyl yellow in alc.                | *    | Blue-violet  | Green       | Still green at pH 3.4, blue-violet at 3.2†                                   |
| 1 part 0.1% methylene blue in alc.               | 3.25 |              |             |                                                                              |
| 1 part 0.14% xylene cyanol FF in alc.            | *    |              |             |                                                                              |
| 1 part 0.1% methyl orange in aq.                 | 3.8  | Violet       | Green       | Color is gray at pH 3.8                                                      |
| 1 part 0.1% methyl orange in aq.                 | *    |              |             |                                                                              |
| 1 part 0.25% indigo carmine in aq.               | 4.1  | Violet       | Green       | Good indicator, especially in artificial light                               |
| 1 part 0.1% methyl orange in aq.                 |      |              |             |                                                                              |
| 1 part 0.1% aniline blue in aq.                  | 4.3  | Violet       | Green       |                                                                              |
| 1 part 0.1% bromcresol green sodium salt in aq.  |      | Orange       | Blue-green  | Yellow at pH 3.5, greenish yellow at 4.0, weakly green at 4.3                |
| 1 part 0.02% methyl orange in aq.                | 4.3  |              |             |                                                                              |
| 3 parts 0.1% bromcresol green in alc.            |      | Wine-red     | Green       | Very sharp color change†                                                     |
| 1 part 0.2% methyl red in alc.                   | 5.1  |              |             |                                                                              |
| 1 part 0.2% methyl red in alc.                   | *    | Red-violet   | Green       | Color is red-violet at pH 5.2, a dirty blue at 5.4, and a dirty green at 5.6 |
| 1 part 0.1% methylene blue in alc.               | 5.4  |              |             |                                                                              |
| 1 part 0.1% chlorphenol red sodium salt in aq.   |      |              |             |                                                                              |
| 1 part 0.1% aniline blue in water                | 5.8  | Green        | Violet      | Pale violet at pH 5.8                                                        |
| 1 part 0.1% bromcresol green sodium salt in aq.  |      | Yellow-green | Blue-violet | Blue-green at pH 5.4, blue at 5.8, blue with a touch of violet at 6.0,       |
| 1 part 0.1% chlorphenol red sodium salt in aq.   | 6.1  |              |             | blue-violet at 6.2                                                           |
| 1 part 0.1% bromcresol purple sodium salt in aq. |      | Yellow       | Violet-blue | Yellow-violet at pH 6.2, violet at 6.6, blue-violet at 6.8                   |
| 1 part 0.1% bromthymol blue sodium salt in aq.   | 6.7  |              |             |                                                                              |
| 2 parts 0.1% bromthymol blue sodium salt in aq.  |      | Violet       | Blue        |                                                                              |
| 1 part 0.1% azolitmin in aq.                     | 6.9  |              |             |                                                                              |

|                                                  |   |      |             |           |                                                                    |
|--------------------------------------------------|---|------|-------------|-----------|--------------------------------------------------------------------|
| 1 part 0.1% neutral red in alc.                  | * |      | Violet-blue | Green     | Violet blue at pH 7.0†                                             |
| 1 part 0.1% methylene blue in alc.               |   | 7.0  |             |           |                                                                    |
| 1 part 0.1% neutral red in alc.                  |   |      | Rose        | Green     | Dirty green at pH 7.4, pale rose at 7.2, clear rose at 7.0         |
| 1 part 0.1% bromthymol blue in alc.              |   | 7.2  |             |           |                                                                    |
| 2 parts 0.1% cyanine in 50% alc.                 |   |      | Yellow      | Violet    | Orange at pH 7.2, beautiful violet at 7.4, color fades on standing |
| 1 part 0.1% phenol red in 50% alc.               |   | 7.3  |             |           |                                                                    |
| 1 part 0.1% bromthymol blue sodium salt in aq.   |   |      | Yellow      | Violet    | Dirty green at pH 7.2, pale violet at 7.4, strong violet at 7.6†   |
| 1 part 0.1% phenol red sodium salt in aq.        |   | 7.5  |             |           |                                                                    |
| 1 part 0.1% cresol red sodium salt in aq.        |   |      | Yellow      | Violet    | Rose at pH 8.2, distinctly violet at 8.4†                          |
| 3 parts 0.1% thymol blue sodium salt in aq.      |   | 8.3  |             |           |                                                                    |
| 2 parts 0.1% $\alpha$ -naphtholphthalein in alc. | * |      | Pale rose   | Violet    | Pale violet at pH 8.2, strong violet at 8.4                        |
| 1 part 0.1% cresol red in alc.                   |   | 8.3  |             |           |                                                                    |
| 1 part 0.1% $\alpha$ -naphtholphthalein in alc.  |   |      | Pale rose   | Violet    | Pale green at pH 8.6, violet at 9.0                                |
| 3 parts 0.1% phenolphthalein in alc.             |   | 8.9  |             |           |                                                                    |
| 1 part 0.1% phenolphthalein in alc.              |   |      | Green       | Violet    | Pale blue at pH 8.8, violet at 9.0                                 |
| 2 parts 0.1% methyl green in alc.                |   | 8.9  |             |           |                                                                    |
| 1 part 0.1% thymol blue in 50% alc.              |   |      | Yellow      | Violet    | From yellow thru green to violet†                                  |
| 3 parts 0.1% phenolphthalein in 50% alc.         |   | 9.0  |             |           |                                                                    |
| 1 part 0.1% phenolphthalein in alc.              |   |      | Colorless   | Violet    | Rose at pH 9.6, violet at 10; sharp color change                   |
| 1 part 0.1% thymolphthalein in alc.              |   | 9.9  |             |           |                                                                    |
| 1 part 0.1% phenolphthalein in alc.              |   |      |             |           |                                                                    |
| 2 parts 0.2% Nile blue in alc.                   |   | 10.0 | Blue        | Red       | Violet at pH 10†                                                   |
| 2 parts 0.1% thymolphthalein in alc.             |   |      |             |           |                                                                    |
| 1 part 0.1% alizarin yellow in alc.              |   | 10.2 | Yellow      | Violet    | Sharp color change                                                 |
| 2 parts 0.2% Nile blue in aq.                    |   |      | Green       | Red-brown |                                                                    |
| 1 part 0.1% alizarin yellow in alc.              |   | 10.8 |             |           |                                                                    |

\* Keep in a dark bottle. † Excellent indicator.



TABLE 8.25 Fluorescent Indicators

| Name                                                   | pH Range     | Color Change<br>Acid to Base | Indicator<br>Solution            |
|--------------------------------------------------------|--------------|------------------------------|----------------------------------|
| Benzoflavine                                           | − 0.3 to 1.7 | Yellow to green              | 1                                |
| 3,6-Dihydroxyphthalimide                               | 0 to 2.4     | Blue to green                | 1                                |
|                                                        | 6.0 to 8.0   | Green to yellow/green        |                                  |
| Eosin (tetrabromofluorescein)                          | 0 to 3.0     | Non-fl to green              | 4, 1%                            |
| 4-Ethoxyacridone                                       | 1.2 to 3.2   | Green to blue                | 1                                |
| 3,6-Tetramethyldiaminoxanthone                         | 1.2 to 3.4   | Green to blue                | 1                                |
| Esculin                                                | 1.5 to 2.0   | Weak blue to strong blue     |                                  |
| Anthranilic acid                                       | 1.5 to 3.0   | Non-fl to light blue         | 2 (50% ethanol)                  |
|                                                        | 4.5 to 6.0   | Light blue to dark blue      |                                  |
|                                                        | 12.5 to 14   | Dark blue to non-fl          |                                  |
| 3-Amino-1-naphthoic acid                               | 1.5 to 3.0   | Non-fl to green              | 2 (as sulfate<br>in 50% ethanol) |
|                                                        | 4.0 to 6.0   | Green to blue                |                                  |
|                                                        | 11.6 to 13.0 | Blue to non-fl               |                                  |
| 1-Naphthylamino-6-sulfonamide<br>(also the 1-, 7-)     | 1.9 to 3.9   | Non-fl to green              | 3                                |
|                                                        | 9.6 to 13.0  | Green to non-fl              |                                  |
| 2-Naphthylamino-6-sulfonamide<br>(also the 2-, 8-)     | 1.9 to 3.9   | Non-fl to dark blue          | 3                                |
|                                                        | 9.6 to 13.0  | Dark blue to non-fl          |                                  |
| 1-Naphthylamino-5-sulfonamide                          | 2.0 to 4.0   | Non-fl to yellow/orange      | 3                                |
|                                                        | 9.5 to 13.0  | Yellow/orange to non-fl      |                                  |
| 1-Naphthoic acid                                       | 2.5 to 3.5   | Non-fl to blue               | 4                                |
| Salicylic acid                                         | 2.5 to 4.0   | Non-fl to dark blue          | 4 (0.5%)                         |
| Phloxin BA extra<br>(tetrachlorotetrabromofluorescein) | 2.5 to 4.0   | Non-fl to dark blue          | 2                                |
| Erythrosin B (tetraiodofluorescein)                    | 2.5 to 4.0   | Non-fl to light green        | 4 (0.2%)                         |
| 2-Naphthylamine                                        | 2.8 to 4.4   | Non-fl to violet             | 1                                |
| Magdala red                                            | 3.0 to 4.0   | Non-fl to purple             |                                  |
| <i>p</i> -Aminophenylbenzenesulfonamide                | 3.0 to 4.0   | Non-fl to light blue         | 3                                |
| 2-Hydroxy-3-naphthoic acid                             | 3.0 to 6.8   | Blue to green                | 4 (0.1%)                         |
| Chromotropic acid                                      | 3.1 to 4.4   | Non-fl to light blue         | 4 (5%)                           |
| 1-Naphthionic acid                                     | 3 to 4       | Non-fl to blue               | 4                                |
|                                                        | 10 to 12     | Blue to yellow-green         |                                  |
| 1-Naphthylamine                                        | 3.4 to 4.8   | Non-fl to blue               | 1                                |
| 5-Aminosalicilic acid                                  | 3.1 to 4.4   | Non-fl to light green        | 1 (0.2% fresh)                   |
| Quinine                                                | 3.0 to 5.0   | Blue to weak violet          | 1 (0.1%)                         |
|                                                        | 9.5 to 10.0  | Weak violet to non-fl        |                                  |
| <i>o</i> -Methoxybenzaldehyde                          | 3.1 to 4.4   | Non-fl to green              | 4 (0.2%)                         |
| <i>o</i> -Phenylenediamine                             | 3.1 to 4.4   | Green to non-fl              | 5                                |
| <i>p</i> -Phenylenediamine                             | 3.1 to 4.4   | Non-fl to orange/yellow      | 5                                |
| Morin (2',4',3,5,7-pentahydroxyflavone)                | 3.1 to 4.4   | Non-fl to green              | 6 (0.2%)                         |
|                                                        | 8 to 9.8     | Green to yellow/green        |                                  |
| Thioflavine S                                          | 3.1 to 4.4   | Dark blue to light blue      | 6 (0.2%)                         |
| Fluorescein                                            | 4.0 to 4.5   | Pink/green to green          | 4 (1%)                           |
| Dichlorofluorescein                                    | 4.0 to 6.6   | Blue green to green          | 1                                |
| $\beta$ -Methylesculetin                               | 4.0 to 6.2   | Non-fl to blue               | 1                                |
|                                                        | 9.0 to 10.0  | Blue to light green          |                                  |
| Quininic acid                                          | 4.0 to 5.0   | Yellow to blue               | 6 (satd)                         |
| $\beta$ -Naphthoquinoline                              | 4.4 to 6.3   | Blue to non-fl               | 3                                |
| Resorufin (7-oxyphenoxazone)                           | 4.4 to 6.4   | Yellow to orange             |                                  |

Indicator solutions: 1, 1% solution in ethanol; 2, 0.1% solution in ethanol; 3, 0.05% solution in 90% ethanol; 4, sodium or potassium salt in distilled water; 5, 0.2% solution in 70% ethanol; 6, distilled water.

**Reference:** G.F. Kirkbright, "Fluorescent Indicators," Chap. 9 in *Indicators*, E. Bishop (ed.), Pergamon Press, Oxford, 1972.

**TABLE 8.25** Fluorescent Indicators (*Continued*)

| Name                                        | pH Range    | Color Change<br>Acid to Base | Indicator<br>Solution                                  |
|---------------------------------------------|-------------|------------------------------|--------------------------------------------------------|
| Acridine                                    | 5.2 to 6.6  | Green to violet              | 2                                                      |
| 3,6-Dihydroxyxanthone                       | 5.4 to 7.6  | Non-fl to blue/violet        | 1                                                      |
| 5,7-Dihydroxy-4-methylcoumarin              | 5.5 to 5.8  | Light blue to dark blue      |                                                        |
| 3,6-Dihydroxyphthalic acid dinitrile        | 5.8 to 8.2  | Blue to green                | 1                                                      |
| 1,4-Dihydroxybenzenedisulfonic acid         | 6 to 7      | Non-fl to light blue         | 4 (0.1%)                                               |
| Luminol                                     | 6 to 7      | Non-fl to blue               |                                                        |
| 2-Naphthol-6-sulfonic acid                  | 5–7 to 8–9  | Non-fl to blue               | 4                                                      |
| Quinoline                                   | 6.2 to 7.2  | Blue to non-fl               | 6 (satd)                                               |
| 1-Naphthol-5-sulfonic acid                  | 6.5 to 7.5  | Non-fl to green              | 6 (satd)                                               |
| Umbelliferone                               | 6.5 to 8.0  | Non-fl to blue               |                                                        |
| Magnesium-8-hydroxyquinolate                | 6.5 to 7.5  | Non-fl to yellow             | 6 (0.1% in<br>0.01 <i>M</i> HCl)                       |
| Orcinaurine                                 | 6.5 to 8.0  | Non-fl to green              | 6 (0.03%)                                              |
| Diazo brilliant yellow                      | 6.5 to 7.5  | Non-fl to blue               |                                                        |
| Coumaric acid                               | 7.2 to 9.0  | Non-fl to green              | 1                                                      |
| $\beta$ -Methylumbelliferone                | >7.0        | Non-fl to blue               | 2 (0.3%)                                               |
| Harmin                                      | 7.2 to 8.9  | Blue to yellow               |                                                        |
| 2-Naphthol-6,8-disulfonic acid              | 7.5 to 9.1  | Blue to light blue           | 4                                                      |
| Salicylaldehyde semicarbazone               | 7.6 to 8.0  | Yellow to blue               | 2                                                      |
| 1-Naphthol-2-sulfonic acid                  | 8.0 to 9.0  | Dark blue to light blue      | 4                                                      |
| Salicylaldehyde acetylhydrazone             | 8.3         | Non-fl to green/blue         | 2                                                      |
| Salicylaldehyde thiosemicarbazone           | 8.4         | Non-fl to blue/green         | 2                                                      |
| 1-Naphthol-4-sulfonic acid                  | 8.2         | Dark blue to light blue      | 4                                                      |
| Naphthol AS                                 | 8.2 to 10.3 | Non-fl to yellow/green       | 4                                                      |
| 2-Naphthol                                  | 8.5 to 9.5  | Non-fl to blue               | 2                                                      |
| Acridine orange                             | 8.4 to 10.4 | Non-fl to yellow/green       | 1                                                      |
| Orcinsulfonephthalein                       | 8.6 to 10.0 | Non-fl to yellow             |                                                        |
| 2-Naphthol-3,6-disulfonic acid              | 9.0 to 9.5  | Dark blue to light blue      | 4                                                      |
| Ethoxyphenylnaphthostilbazonium chloride    | 9 to 11     | Green to non-fl              | 1                                                      |
| <i>o</i> -Hydroxyphenylbenzothiazole        | 9.3         | Non-fl to blue green         | 2                                                      |
| <i>o</i> -Hydroxyphenylbenzoxazole          | 9.3         | Non-fl to blue/violet        | 2                                                      |
| <i>o</i> -Hydroxyphenylbenzimidazole        | 9.9         | Non-fl to blue/violet        | 2                                                      |
| Coumarin                                    | 9.5 to 10.5 | Non-fl to light green        |                                                        |
| 6,7-Dimethoxyisoquinoline-1-carboxylic acid | 9.5 to 11.0 | Yellow to blue               | 0.1% in glycerine/<br>ethanol/water in<br>2:2:18 ratio |
| 1-Naphthylamino-4-sulfonamide               | 9.5 to 13.0 | Dark blue to white/blue      | 3                                                      |

**TABLE 8.26** Selected List of Oxidation-Reduction Indicators

| Name                                                            | Reduction Potential<br>(30°C) in Volts at                                                                                                        |        | Suitable<br>pH Range | Color Change<br>Upon Oxidation |
|-----------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|--------|----------------------|--------------------------------|
|                                                                 | pH = 0                                                                                                                                           | pH = 7 |                      |                                |
| Bis(5-bromo-1,10-phenanthroline)<br>ruthenium(II) dinitrate     | 1.41*                                                                                                                                            |        |                      | Red to faint blue              |
| Tris(5-nitro-1,10-phenanthroline)<br>iron(II) sulfate           | 1.25*                                                                                                                                            |        |                      | Red to faint blue              |
| Iron(II)-2,2',2''-tripyridine sulfate                           | 1.25*                                                                                                                                            |        |                      | Pink to faint blue             |
| Tris(4,7-diphenyl-1,10-phenanthroline)<br>iron(II) disulfate    | 1.13 (4.6 M H <sub>2</sub> SO <sub>4</sub> )*<br>0.87 (1.0 M H <sub>2</sub> SO <sub>4</sub> )*                                                   |        |                      | Red to faint blue              |
| <i>o,m'</i> -Diphenylaminedicarboxylic acid                     | 1.12                                                                                                                                             |        |                      | Colorless to blue-violet       |
| Setopaline                                                      | 1.06 ( <i>trans</i> )†                                                                                                                           |        |                      | Yellow to orange               |
| <i>p</i> -Nitrodiphenylamine                                    | 1.06                                                                                                                                             |        |                      | Colorless to violet            |
| Tris(1,10-phenanthroline)-iron(II) sulfate                      | 1.06 (1.00 M H <sub>2</sub> SO <sub>4</sub> )*<br>1.00 (3.0 M H <sub>2</sub> SO <sub>4</sub> )*<br>0.89 (6.0 M H <sub>2</sub> SO <sub>4</sub> )* |        |                      | Red to faint blue              |
| Setoglaucine O                                                  | 1.01 ( <i>trans</i> )†                                                                                                                           |        |                      | Yellow-green to yellow-red     |
| Xylene cyanole FF                                               | 1.00 ( <i>trans</i> )†                                                                                                                           |        |                      | Yellow-green to pink           |
| Erioglaucine A                                                  | 1.00 ( <i>trans</i> )†                                                                                                                           |        |                      | Green-yellow to bluish red     |
| Eriogreen                                                       | 0.99 ( <i>trans</i> )†                                                                                                                           |        |                      | Green-yellow to orange         |
| Tris(2,2'-bipyridine)-iron(II)<br>hydrochloride                 | 0.97*                                                                                                                                            |        |                      | Red to faint blue              |
| 2-Carboxydiphenylamine [ <i>N</i> -phenyl-<br>anthranilic acid] | 0.94                                                                                                                                             |        |                      | Colorless to pink              |
| Benzidine dihydrochloride                                       | 0.92                                                                                                                                             |        |                      | Colorless to blue              |
| <i>o</i> -Toluidine                                             | 0.87                                                                                                                                             |        |                      | Colorless to blue              |
| Bis(1,10-phenanthroline)-osmium(II)<br>perchlorate              | 0.859 (0.1 M H <sub>2</sub> SO <sub>4</sub> )                                                                                                    |        |                      | Green to pink                  |
| Diphenylamine-4-sulfonate (Na salt)                             | 0.85                                                                                                                                             |        |                      | Colorless to violet            |

|                                                                                     |        |        |          |                          |
|-------------------------------------------------------------------------------------|--------|--------|----------|--------------------------|
| 3,3'-Dimethoxybenzidine dihydrochloride<br>[o-dianisidine]                          | 0.85   |        |          | Colorless to red         |
| Ferrocypen                                                                          | 0.81   |        |          | Yellow to violet         |
| 4'-Ethoxy-2,4-diaminoazobenzene                                                     | 0.76   |        |          | Red to pale yellow       |
| N,N-Diphenylbenzidine                                                               | 0.76   |        |          | Colorless to violet      |
| Diphenylamine                                                                       | 0.76   |        |          | Colorless to violet      |
| N,N-Dimethyl-p-phenylenediamine                                                     | 0.76   |        |          | Colorless to red         |
| Variamine blue B hydrochloride                                                      | 0.712‡ | 0.310  | 1.5–6.3  | Colorless to blue        |
| N-Phenyl-1,2,4-benzenetriamine                                                      | 0.70   |        |          | Colorless to red         |
| Bindschedler's green                                                                | 0.680‡ | 0.224  | 2–9.5    |                          |
| 2,6-Dichloroindophenol (Na salt)                                                    | 0.668‡ | 0.217  | 6.3–11.4 | Colorless to blue        |
| 2,6-Dibromophenolindophenol                                                         | 0.668‡ | 0.216  | 7.0–12.3 | Colorless to blue        |
| Brilliant cresyl blue [3-amino-9-dimethyl-<br>amino-10-methylphenoxyazine chloride] | 0.583  | 0.047  | 0–11     | Colorless to blue        |
| Iron(II)-tetrapyridine chloride                                                     | 0.59   |        |          | Red to faint blue        |
| Thionine [Lauth's violet]                                                           | 0.563‡ | 0.064  | 1–13     | Colorless to violet      |
| Starch (soluble potato, I <sub>3</sub> <sup>-</sup> present)                        | 0.54   |        |          | Colorless to blue        |
| Gallocyanine (25°C)                                                                 |        | 0.021  |          | Colorless to violet-blue |
| Methylene blue                                                                      | 0.532‡ | 0.011  | 1–13     | Colorless to blue        |
| Nile blue A [aminonaphthodiethylamino-<br>phenoxazine sulfate]                      | 0.406‡ | –0.119 | 1.4–12.3 | Colorless to blue        |
| Indigo-5,5',7,7'-tetrasulfonic acid<br>(Na salt)                                    | 0.365‡ | –0.046 | <9       | Colorless to blue        |
| Indigo-5,5',7-trisulfonic acid (Na salt)                                            | 0.332‡ | –0.081 | <9       | Colorless to blue        |
| Indigo-5,5'-disulfonic acid (Na salt)                                               | 0.291‡ | –0.125 | <9       | Colorless to blue        |
| Phenosafranine                                                                      | 0.280‡ | –0.252 | 1–11     | Colorless to violet-blue |
| Indigo-5-monosulfonic acid (Na salt)                                                | 0.262‡ | –0.157 | <9       | Colorless to blue        |
| Safranin T                                                                          | 0.24‡  | –0.289 | 1–12     | Colorless to violet-blue |
| Bis(dimethylglyoximate)-iron(II) chloride                                           | 0.155  |        | 6–10     | Red to colorless         |
| Induline scarlet                                                                    | 0.047‡ | –0.299 | 3–8.6    | Colorless to red         |
| Neutral red                                                                         |        | –0.323 | 2–11     | Colorless to red-violet  |

\* Transition point is at higher potential than the tabulated formal potential because the molar absorptivity of the reduced form is very much greater than that of the oxidized form.

† *Trans* = first noticeable color transition; often 60 mV less than  $E^\circ$

‡ Values of  $E^\circ$  are obtained by extrapolation from measurements in weakly acid or weakly alkaline systems.

8.6 ELECTRODE POTENTIALS

TABLE 8.27 Potentials of the Elements and Their Compounds at 25°C

Standard potentials are tabulated except when a solution composition is stated; the latter are formal potentials and the concentrations are in mol/liter.

| Half-reaction                                                                              | Standard or formal potential | Solution composition |
|--------------------------------------------------------------------------------------------|------------------------------|----------------------|
| <b>Actinium</b>                                                                            |                              |                      |
| $\text{Ac}^{3+} + 3e^- = \text{Ac}$                                                        | -2.13                        |                      |
| <b>Aluminum</b>                                                                            |                              |                      |
| $\text{Al}^{3+} + 3e^- = \text{Al}$                                                        | -1.676                       |                      |
| $\text{AlF}_6^{3-} + 3e^- = \text{Al} + 6\text{F}^-$                                       | -2.07                        |                      |
| $\text{Al}(\text{OH})_4^- + 3e^- = \text{Al} + 4\text{OH}^-$                               | -2.310                       |                      |
| <b>Americium</b>                                                                           |                              |                      |
| $\text{AmO}_2^{2+} + 4\text{H}^+ + 2e^- = \text{Am}^{4+} + 2\text{H}_2\text{O}$            | 1.20                         |                      |
| $\text{AmO}_2^{2+} + e^- = \text{AmO}_2^+$                                                 | 1.59                         |                      |
| $\text{AmO}_2^+ + 4\text{H}^+ + e^- = \text{Am}^{4+} + 2\text{H}_2\text{O}$                | 0.82                         |                      |
| $\text{AmO}_2^+ + 4\text{H}^+ + 2e^- = \text{Am}^{3+} + 2\text{H}_2\text{O}$               | 1.72                         |                      |
| $\text{Am}^{4+} + e^- = \text{Am}^{3+}$                                                    | 2.62                         |                      |
| $\text{Am}^{4+} + 4e^- = \text{Am}$                                                        | -0.90                        |                      |
| $\text{Am}^{3+} + 3e^- = \text{Am}$                                                        | -2.07                        |                      |
| <b>Antimony</b>                                                                            |                              |                      |
| $\text{Sb}(\text{OH})_4^- + 2e^- = \text{SbO}_2^- + 2\text{OH}^- + 2\text{H}_2\text{O}$    | -0.465                       | 1 NaOH               |
| $\text{SbO}_2^- + 2\text{H}_2\text{O} + 3e^- = \text{Sb} + 4\text{OH}^-$                   | 0.639                        | 1 NaOH               |
| $\text{Sb} + 3\text{H}_2\text{O} + 3e^- = \text{SbH}_3 + 3\text{OH}^-$                     | -1.338                       | 1 NaOH               |
| $\text{Sb}_2\text{O}_5 + 6\text{H}^+ + 4e^- = 2\text{SbO}^+ + 3\text{H}_2\text{O}$         | 0.605                        |                      |
| $\text{Sb}_2\text{O}_5 + 4\text{H}^+ + 4e^- = \text{Sb}_2\text{O}_3 + 2\text{H}_2\text{O}$ | 0.699                        |                      |
| $\text{Sb}_2\text{O}_5 + 2\text{H}^+ + 2e^- = \text{Sb}_2\text{O}_4 + \text{H}_2\text{O}$  | 1.055                        |                      |
| $\text{Sb}_2\text{O}_4 + 2\text{H}^+ + 2e^- = \text{Sb}_2\text{O}_3 + \text{H}_2$          | 0.342                        |                      |
| $\text{SbO}^+ + 2\text{H}^+ + 3e^- = \text{Sb} + \text{H}_2\text{O}$                       | 0.204                        |                      |
| $\text{Sb} + 3\text{H}^+ + 3e^- = \text{SbH}_3$                                            | -0.510                       |                      |
| <b>Arsenic</b>                                                                             |                              |                      |
| $\text{H}_3\text{AsO}_4 + 2\text{H}^+ + 2e^- = \text{HAsO}_2 + 2\text{H}_2\text{O}$        | 0.560                        |                      |
| $\text{HAsO}_2 + 3\text{H}^+ + 3e^- = \text{As} + 2\text{H}_2\text{O}$                     | 0.240                        |                      |
| $\text{As} + 3\text{H}^+ + 3e^- = \text{AsH}_3$                                            | -0.225                       |                      |
| $\text{AsO}_4^{3-} + 2\text{H}^+ + 2e^- = \text{AsO}_2^- + 4\text{OH}^-$                   | -0.67                        |                      |
| $\text{AsO}_2^- + 2\text{H}_2\text{O} + 3e^- = \text{As} + 4\text{OH}^-$                   | -0.68                        |                      |
| $\text{As} + 3\text{H}_2\text{O} + 3e^- = \text{AsH}_3 + 3\text{OH}^-$                     | -1.37                        |                      |
| <b>Astatine</b>                                                                            |                              |                      |
| $\text{HAtO}_3 + 4\text{H}^+ + 4e^- = \text{HAtO} + 2\text{H}_2$                           | ca. 1.4                      |                      |
| $2\text{HAtO} + 2\text{H}^+ + 2e^- = \text{At}_2 + 2\text{H}_2\text{O}$                    | ca. 0.7                      |                      |
| $\text{At}_2 + 2e^- = 2\text{At}^-$                                                        | 0.20                         |                      |
| <b>Barium</b>                                                                              |                              |                      |
| $\text{BaO}_2 + 4\text{H}^+ + 2e^- = \text{Ba}^{2+} + 2\text{H}_2\text{O}$                 | 2.365                        |                      |
| $\text{Ba}^{2+} + 2e^- = \text{Ba}$                                                        | -2.92                        |                      |

Source: A. J. Bard, R. Parsons, and J. Jordan (eds.), *Standard Potentials in Aqueous Solution* (prepared under the auspices of the International Union of Pure and Applied Chemistry), Marcel Dekker, New York, 1985; G. Charlot et al., *Selected Constants: Oxidation-Reduction Potentials of Inorganic Substances in Aqueous Solution*, Butterworths, London, 1971.

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                     | Standard<br>or formal<br>potential | Solution<br>composition |
|---------------------------------------------------------------------------------------------------|------------------------------------|-------------------------|
| <b>Berkelium</b>                                                                                  |                                    |                         |
| $\text{Bk}^{4+} + 4e^- = \text{Bk}$                                                               | -1.05                              |                         |
| $\text{Bk}^{4+} + e^- = \text{Bk}^{3+}$                                                           | 1.67                               |                         |
| $\text{Bk}^{3+} + 3e^- = \text{Bk}$                                                               | -2.01                              |                         |
| <b>Beryllium</b>                                                                                  |                                    |                         |
| $\text{Be}^{2+} + 2e^- = \text{Be}$                                                               | -1.99                              |                         |
| <b>Bismuth</b>                                                                                    |                                    |                         |
| $\text{Bi}_2\text{O}_4$ (bismuthate) + $4\text{H}^+ + 2e^- = 2\text{BiO}^+ + 2\text{H}_2\text{O}$ | 1.59                               |                         |
| $\text{Bi}^{3+} + 3e^- = \text{Bi}$                                                               | 0.317                              |                         |
| $\text{Bi} + 3\text{H}^+ + 3e^- = \text{BiH}_3$                                                   | -0.97                              |                         |
| $\text{BiCl}_4^- + 3e^- = \text{Bi} + 4\text{Cl}^-$                                               | 0.199                              |                         |
| $\text{BiBr}_4^- + 3e^- = \text{Bi} + 4\text{Br}^-$                                               | 0.168                              |                         |
| $\text{BiOCl} + 2\text{H}^+ + 3e^- = \text{Bi} + \text{H}_2\text{O} + \text{Cl}^-$                | 0.170                              |                         |
| <b>Boron</b>                                                                                      |                                    |                         |
| $\text{B}(\text{OH})_3 + 3\text{H}^+ + 3e^- = \text{B} + 3\text{H}_2\text{O}$                     | -0.890                             |                         |
| $\text{BO}_2^- + 6\text{H}_2\text{O} + 8e^- = \text{BH}_3^- + 8\text{OH}^-$                       | -1.241                             |                         |
| $\text{B}(\text{OH})_4^- + 3e^- = \text{B} + 4\text{OH}^-$                                        | -1.811                             |                         |
| <b>Bromine</b>                                                                                    |                                    |                         |
| $\text{BrO}_4^- + 2\text{H}^+ + 2e^- = \text{BrO}_3^- + \text{H}_2\text{O}$                       | 1.853                              |                         |
| $\text{BrO}_3^- + 6\text{H}^+ + 6e^- = \text{Br}^- + 3\text{H}_2\text{O}$                         | 1.478                              |                         |
| $\text{BrO}_3^- + 5\text{H}^+ + 4e^- = \text{HBrO} + 2\text{H}_2\text{O}$                         | 1.444                              |                         |
| $2\text{BrO}_3^- + 12\text{H}^+ + 10e^- = \text{Br}_2 + 6\text{H}_2\text{O}$                      | 1.5                                |                         |
| $2\text{HBrO} + 2\text{H}^+ + 2e^- = \text{Br}_2 + 2\text{H}_2\text{O}$                           | 1.604                              |                         |
| $\text{HBrO} + \text{H}^+ + 2e^- = \text{Br}^- + \text{H}_2\text{O}$                              | 1.341                              |                         |
| $\text{BrO}^- + \text{H}_2\text{O} + 2e^- = \text{Br}^- + 2\text{OH}^-$                           | 0.76                               | 1 NaOH                  |
| $\text{Br}_3^- + 2e^- = 3\text{Br}^-$                                                             | 1.050                              |                         |
| $\text{Br}_2(\text{aq}) + 2e^- = 2\text{Br}^-$                                                    | 1.087                              |                         |
| <b>Cadmium</b>                                                                                    |                                    |                         |
| $\text{Cd}^{2+} + 2e^- = \text{Cd}$                                                               | -0.403                             |                         |
| $\text{Cd}^{2+} + \text{Hg} + 2e^- = \text{Cd}(\text{Hg})$                                        | -0.352                             |                         |
| $\text{CdCl}_4^{2-} + 2e^- = \text{Cd} + 4\text{Cl}^-$                                            | -0.453                             |                         |
| $\text{Cd}(\text{CN})_4^{2-} + 2e^- = \text{Cd} + 4\text{CN}^-$                                   | -0.943                             |                         |
| $\text{Cd}(\text{NH}_3)_4^{2+} + 2e^- = \text{Cd} + 4\text{NH}_3$                                 | -0.622                             |                         |
| $\text{Cd}(\text{OH})_4^{2-} + 2e^- = \text{Cd} + 4\text{OH}^-$                                   | -0.670                             |                         |
| <b>Calcium</b>                                                                                    |                                    |                         |
| $\text{CaO}_2 + 4\text{H}^+ + 2e^- = \text{Ca}^{2+} + \text{H}_2\text{O}$                         | 2.224                              |                         |
| $\text{Ca}^{2+} + 2e^- = \text{Ca}$                                                               | -2.84                              |                         |
| $\text{Ca} + 2\text{H}^+ + 2e^- = \text{CaH}_2$                                                   | 0.776                              |                         |
| <b>Californium</b>                                                                                |                                    |                         |
| $\text{Cf}^{3+} + 3e^- = \text{Cf}$                                                               | -1.93                              |                         |
| $\text{Cf}^{3+} + e^- = \text{Cf}^{2+}$                                                           | -1.6                               |                         |
| $\text{Cf}^{2+} + 2e^- = \text{Cf}$                                                               | -2.1                               |                         |
| <b>Carbon</b>                                                                                     |                                    |                         |
| $\text{CO}_2 + 2\text{H}^+ + 2e^- = \text{CO} + \text{H}_2\text{O}$                               | -0.106                             |                         |
| $\text{CO}_2 + 2\text{H}^+ + 2e^- = \text{HCOOH}$                                                 | -0.20                              |                         |
| $2\text{CO}_2 + 2\text{H}^+ + 2e^- = \text{H}_2\text{C}_2\text{O}_4$                              | -0.481                             |                         |
| $\text{C}_2\text{O}_4^{2-} + 2\text{H}^+ + 2e^- = 2\text{HCOO}^-$                                 | 0.145                              |                         |
| $\text{HCOOH} + 2\text{H}^+ + 2e^- = \text{HCHO} + \text{H}_2\text{O}$                            | 0.034                              |                         |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                              | Standard or formal potential | Solution composition        |
|--------------------------------------------------------------------------------------------|------------------------------|-----------------------------|
| $\text{C}_2\text{N}_2 + 2\text{H}^+ + 2e^- = 2\text{HCN}$                                  | 0.373                        |                             |
| $\text{HCNO} + 2\text{H}^+ + 2e^- = \text{CO} + \text{H}_2\text{O}$                        | 0.330                        |                             |
| $\text{HCHO} + 2\text{H}^+ + 2e^- = \text{CH}_3\text{OH}$                                  | 0.2323                       |                             |
| $\text{CNO}^- + \text{H}_2\text{O} + 2e^- = \text{CN}^- + 2\text{OH}^-$                    | -0.97                        |                             |
| <b>Cerium</b>                                                                              |                              |                             |
| $\text{Ce(IV)} + e^- = \text{Ce(III)}$                                                     | 1.70                         | 1 $\text{HClO}_4$           |
|                                                                                            | 1.61                         | 1 $\text{HNO}_3$            |
|                                                                                            | 1.44                         | 0.5 $\text{H}_2\text{SO}_4$ |
|                                                                                            | 1.28                         | 1 $\text{HCl}$              |
| $\text{Ce}^{3+} + 3e^- = \text{Ce}$                                                        | -2.34                        |                             |
| <b>Cesium</b>                                                                              |                              |                             |
| $\text{Cs}^+ + e^- = \text{Cs}$                                                            | -2.923                       |                             |
| $\text{Cs}^+ + \text{Hg} + e^- = \text{Cs(Hg)}$                                            | -1.78                        |                             |
| <b>Chlorine</b>                                                                            |                              |                             |
| $\text{ClO}_4^- + 2\text{H}^+ + 2e^- = \text{ClO}_3^- + \text{H}_2\text{O}$                | 1.201                        |                             |
| $2\text{ClO}_4^- + 16\text{H}^+ + 14e^- = \text{Cl}_2 + 8\text{H}_2\text{O}$               | 1.392                        |                             |
| $\text{ClO}_4^- + 8\text{H}^+ + 8e^- = \text{Cl}^- + 4\text{H}_2\text{O}$                  | 1.388                        |                             |
| $\text{ClO}_3^- + 2\text{H}^+ + e^- = \text{ClO}_2(\text{g}) + \text{H}_2\text{O}$         | 1.175                        |                             |
| $\text{ClO}_3^- + 3\text{H}^+ + 2e^- = \text{HClO}_2 + \text{H}_2\text{O}$                 | 1.181                        |                             |
| $2\text{ClO}_3^- + 12\text{H}^+ + 10e^- = \text{Cl}_2 + 6\text{H}_2\text{O}$               | 1.468                        |                             |
| $\text{ClO}_3^- + 6\text{H}^+ + 6e^- = \text{Cl}^- + 3\text{H}_2\text{O}$                  | 1.45                         |                             |
| $\text{ClO}_2(\text{g}) + \text{H}^+ + e^- = \text{HClO}_2$                                | 1.188                        |                             |
| $\text{HClO}_2 + 2\text{H}^+ + 2e^- = \text{HClO} + \text{H}_2\text{O}$                    | 1.64                         |                             |
| $\text{HClO}_2 + 3\text{H}^+ + 4e^- = \text{Cl}^- + 2\text{H}_2\text{O}$                   | 1.584                        |                             |
| $2\text{HClO}_2 + 6\text{H}^+ + 6e^- = \text{Cl}_2(\text{g}) + 4\text{H}_2\text{O}$        | 1.659                        |                             |
| $2\text{ClO}^- + 2\text{H}_2\text{O} + 2e^- = \text{Cl}_2(\text{g}) + 4\text{OH}^-$        | 0.421                        | 1 $\text{NaOH}$             |
| $\text{ClO}^- + \text{H}_2\text{O} + 2e^- = \text{Cl}^- + 2\text{OH}^-$                    | 0.890                        | 1 $\text{NaOH}$             |
| $\text{Cl}_3^- + 2e^- = 3\text{Cl}^-$                                                      | 1.415                        |                             |
| $\text{Cl}_2(\text{aq}) + 2e^- = 2\text{Cl}^-$                                             | 1.396                        |                             |
| <b>Chromium</b>                                                                            |                              |                             |
| $\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6e^- = 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$ | 1.36                         |                             |
|                                                                                            | 1.15                         | 0.1 $\text{H}_2\text{SO}_4$ |
|                                                                                            | 1.03                         | 1 $\text{HClO}_4$           |
| $\text{CrO}_4^{2-} + 4\text{H}_2\text{O} + 3e^- = \text{Cr(OH)}_4^- + 4\text{OH}^-$        | -0.13                        | 1 $\text{NaOH}$             |
| $\text{Cr}^{3+} + e^- = \text{Cr}^{2+}$                                                    | -0.424                       |                             |
| $\text{Cr}^{3+} + 3e^- = \text{Cr}$                                                        | -0.74                        |                             |
| $\text{Cr}^{2+} + 2e^- = \text{Cr}$                                                        | 0.90                         |                             |
| <b>Cobalt</b>                                                                              |                              |                             |
| $\text{CoO}_2 + 4\text{H}^+ + e^- = \text{Co}^{3+} + 2\text{H}_2\text{O}$                  | 1.416                        |                             |
| $\text{Co(H}_2\text{O)}_6^{3+} + e^- = \text{Co(H}_2\text{O)}_6^{2+}$                      | 1.92                         |                             |
| $\text{Co(NH}_3)_6^{3+} + e^- = \text{Co(NH}_3)_6^{2+}$                                    | 0.058                        | 7 $\text{NH}_3$             |
| $\text{Co(OH)}_3 + e^- = \text{Co(OH)}_2 + \text{OH}^-$                                    | 0.17                         |                             |
| $\text{Co(en)}_3^{3+} + e^- = \text{Co(en)}_3^{2+}$ [en = ethylenediamine]                 | -0.2                         | 0.1 en                      |
| $\text{Co(CN)}_6^{3-} + e^- = \text{Co(CN)}_6^{2-} + \text{CN}^-$                          | -0.8                         | 0.8 $\text{KOH}$            |
| $\text{Co}^{2+} + 2e^- = \text{Co}$                                                        | -0.277                       |                             |
| $\text{Co(NH}_3)_6^{2+} + 2e^- = \text{Co} + 6\text{NH}_3$                                 | -0.422                       |                             |
| $[\text{Co(CO)}_4]_2 + 2e^- = 2\text{Co(CO)}_4^-$                                          | -0.40                        |                             |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                           | Standard or formal potential | Solution composition |
|-------------------------------------------------------------------------|------------------------------|----------------------|
| <b>Copper</b>                                                           |                              |                      |
| $\text{Cu}^{2+} + 2e^- = \text{Cu}$                                     | 0.340                        |                      |
| $\text{Cu}^{2+} + e^- = \text{Cu}^+$                                    | 0.159                        |                      |
| $\text{Cu}^+ + e^- = \text{Cu}$                                         | 0.520                        |                      |
| $\text{Cu}^{2+} + \text{Cl}^- + e^- = \text{CuCl}$                      | 0.559                        |                      |
| $\text{Cu}^{2+} + 2\text{Br}^- + e^- = \text{CuBr}_2^-$                 | 0.52                         | 1 KBr                |
| $\text{Cu}^{2+} + \text{I}^- + e^- = \text{CuI}$                        | 0.86                         |                      |
| $\text{Cu}^{2+} + 2\text{CN}^- + e^- = \text{Cu(CN)}_2^-$               | 1.12                         |                      |
| $\text{Cu(NH}_3)_3^+ + e^- = \text{Cu(NH}_3)_2^+ + 2\text{NH}_3$        | 0.10                         | 1 $\text{NH}_3$      |
| $\text{Cu(en)}_2^+ + e^- = \text{Cu(en)}^+ + \text{en}$                 | -0.35                        |                      |
| $\text{Cu(CN)}_2^- + e^- = \text{Cu} + 2\text{CN}^-$                    | -0.44                        |                      |
| $\text{CuCl}_2^- + e^- = \text{Cu} + 3\text{Cl}^-$                      | 0.178                        | 1 HCl                |
| $\text{Cu(NH}_3)_2^+ + e^- = \text{Cu} + 2\text{NH}_3$                  | -0.100                       |                      |
| <b>Curium</b>                                                           |                              |                      |
| $\text{Cm}^{4+} + e^- = \text{Cm}^{3+}$                                 | 3.2                          | 1 $\text{HClO}_4$    |
| $\text{Cm}^{3+} + 3e^- = \text{Cm}$                                     | -2.06                        |                      |
| <b>Dysprosium</b>                                                       |                              |                      |
| $\text{Dy}^{3+} + 3e^- = \text{Dy}$                                     | -2.29                        |                      |
| $\text{Dy}^{3+} + e^- = \text{Dy}^{2+}$                                 | -2.5                         |                      |
| $\text{Dy}^{2+} + 2e^- = \text{Dy}$                                     | -2.2                         |                      |
| <b>Einsteinium</b>                                                      |                              |                      |
| $\text{Es}^{3+} + 3e^- = \text{Es}$                                     | -2.0                         |                      |
| $\text{Es}^{3+} + e^- = \text{Es}^{2+}$                                 | -1.5                         |                      |
| $\text{Es}^{2+} + 2e^- = \text{Es}$                                     | -2.2                         |                      |
| <b>Erbium</b>                                                           |                              |                      |
| $\text{Er}^{3+} + 3e^- = \text{Er}$                                     | -2.32                        |                      |
| <b>Europium</b>                                                         |                              |                      |
| $\text{Eu}^{3+} + 3e^- = \text{Eu}$                                     | -1.99                        |                      |
| $\text{Eu}^{3+} + e^- = \text{Eu}^{2+}$                                 | -0.35                        |                      |
| $\text{Eu}^{2+} + 2e^- = \text{Eu}$                                     | -2.80                        |                      |
| <b>Fermium</b>                                                          |                              |                      |
| $\text{Fm}^{3+} + 3e^- = \text{Fm}$                                     | -1.96                        |                      |
| $\text{Fm}^{3+} + e^- = \text{Fm}^{2+}$                                 | -1.15                        |                      |
| $\text{Fm}^{2+} + 2e^- = \text{Fm}$                                     | -2.37                        |                      |
| <b>Fluorine</b>                                                         |                              |                      |
| $\text{F}_2 + 2\text{H}^+ + 2e^- = 2\text{HF}$                          | 3.053                        |                      |
| $\text{F}_2 + \text{H}^+ + 2e^- = \text{HF}_2^-$                        | 2.979                        |                      |
| $\text{F}_2 + 2e^- = 2\text{F}^-$                                       | 2.87                         |                      |
| $\text{OF}_2 + 3\text{H}^+ + 4e^- = \text{HF}_2^- + \text{H}_2\text{O}$ | 2.209                        |                      |
| <b>Francium</b>                                                         |                              |                      |
| $\text{Fr}^+ + e^- = \text{Fr}$                                         | ca. -2.9                     |                      |
| <b>Gadolinium</b>                                                       |                              |                      |
| $\text{Gd}^{3+} + 3e^- = \text{Gd}$                                     | -2.28                        |                      |
| <b>Gallium</b>                                                          |                              |                      |
| $\text{Ga}^{3+} + 3e^- = \text{Ga}$                                     | -0.529                       |                      |
| $\text{Ga}^{3+} + e^- = \text{Ga}^{2+}$                                 | -0.65                        |                      |
| $\text{Ga}^{2+} + 2e^- = \text{Ga}$                                     | -0.45                        |                      |



**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                            | Standard<br>or formal<br>potential | Solution<br>composition |
|----------------------------------------------------------------------------------------------------------|------------------------------------|-------------------------|
| <b>Germanium</b>                                                                                         |                                    |                         |
| $\text{GeO}_2(\text{tetr}) + 2\text{H}^+ + 2\text{e}^- = \text{GeO}(\text{yellow}) + \text{H}_2\text{O}$ | -0.255                             |                         |
| $\text{GeO}_2(\text{tetr}) + 4\text{H}^+ + 2\text{e}^- = \text{Ge}^{2+} + 2\text{H}_2\text{O}$           | -0.210                             |                         |
| $\text{GeO}_2(\text{hex}) + 4\text{H}^+ + 2\text{e}^- = \text{Ge}^{2+} + 2\text{H}_2\text{O}$            | -0.132                             |                         |
| $\text{H}_2\text{GeO}_3 + 4\text{H}^+ + 4\text{e}^- = \text{Ge} + 3\text{H}_2\text{O}$                   | 0.012                              |                         |
| $\text{Ge}^{4+} + 2\text{e}^- = \text{Ge}^{2+}$                                                          | 0.0                                |                         |
| $\text{Ge}^{2+} + 2\text{e}^- = \text{Ge}$                                                               | 0.247                              |                         |
| $\text{GeO} + 2\text{H}^+ + 2\text{e}^- = \text{Ge} + \text{H}_2\text{O}$                                | -0.255                             |                         |
| $\text{Ge} + 4\text{H}^+ + 4\text{e}^- = \text{GeH}_4$                                                   | -0.29                              |                         |
| <b>Gold</b>                                                                                              |                                    |                         |
| $\text{Au}^{3+} + 3\text{e}^- = \text{Au}$                                                               | 1.52                               |                         |
| $\text{Au}^{3+} + 2\text{e}^- = \text{Au}^+$                                                             | 1.36                               |                         |
| $\text{Au}^+ + \text{e}^- = \text{Au}$                                                                   | 1.83                               |                         |
| $\text{AuCl}_4^- + 2\text{e}^- = \text{AuCl}_2^- + 2\text{Cl}^-$                                         | 0.926                              |                         |
| $\text{AuBr}_4^- + 2\text{e}^- = \text{AuBr}_2^- + 2\text{Br}^-$                                         | 0.802                              |                         |
| $\text{Au}(\text{SCN})_4^- + 2\text{e}^- = \text{Au}(\text{SCN})_2^- + 2\text{SCN}^-$                    | 0.623                              |                         |
| $\text{AuBr}_4^- + 3\text{e}^- = \text{Au} + 4\text{Br}^-$                                               | 0.854                              |                         |
| $\text{AuCl}_4^- + 3\text{e}^- = \text{Au} + 4\text{Cl}^-$                                               | 1.002                              |                         |
| $\text{Au}(\text{SCN})_4^- + 3\text{e}^- = \text{Au} + 4\text{SCN}^-$                                    | 0.662                              |                         |
| $\text{Au}(\text{OH})_3 + 3\text{H}^+ + 3\text{e}^- = \text{Au} + 3\text{H}_2\text{O}$                   | 1.45                               |                         |
| $\text{AuBr}_2^- + \text{e}^- = \text{Au} + 2\text{Br}^-$                                                | 0.960                              |                         |
| $\text{AuCl}_2^- + \text{e}^- = \text{Au} + 2\text{Cl}^-$                                                | 1.15                               |                         |
| $\text{AuI}_2^- + \text{e}^- = \text{Au} + 2\text{I}^-$                                                  | 0.576                              |                         |
| $\text{Au}(\text{CN})_2^- + \text{e}^- = \text{Au} + 2\text{CN}^-$                                       | -0.596                             |                         |
| $\text{Au}(\text{SCN})_2 + \text{e}^- = \text{Au} + 2\text{SCN}^-$                                       | 0.69                               |                         |
| <b>Hafnium</b>                                                                                           |                                    |                         |
| $\text{Hf}^{4+} + 4\text{e}^- = \text{Hf}$                                                               | -1.70                              |                         |
| $\text{HfO}_2 + 4\text{H}^+ + 4\text{e}^- = \text{Hf} + 2\text{H}_2\text{O}$                             | -1.57                              |                         |
| <b>Holmium</b>                                                                                           |                                    |                         |
| $\text{Ho}^{3+} + 3\text{e}^- = \text{Ho}$                                                               | -2.23                              |                         |
| <b>Hydrogen</b>                                                                                          |                                    |                         |
| $2\text{H}^+ + 2\text{e}^- = \text{H}_2$                                                                 | 0.0000                             |                         |
| $2\text{D}^+ + 2\text{e}^- = \text{D}_2$                                                                 | 0.029                              |                         |
| $2\text{H}_2\text{O} + 2\text{e}^- = \text{H}_2 + 2\text{OH}^-$                                          | -0.828                             |                         |
| <b>Indium</b>                                                                                            |                                    |                         |
| $\text{In}^{3+} + 3\text{e}^- = \text{In}$                                                               | -0.338                             |                         |
| $\text{In}^{3+} + 2\text{e}^- = \text{In}^+$                                                             | -0.444                             |                         |
| $\text{In}^+ + \text{e}^- = \text{In}$                                                                   | -0.126                             |                         |
| <b>Iodine</b>                                                                                            |                                    |                         |
| $\text{H}_5\text{IO}_6 + \text{H}^+ + 2\text{e}^- = \text{IO}_3^- + 3\text{H}_2\text{O}$                 | 1.603                              |                         |
| $\text{IO}_3^- + 5\text{H}^+ + 4\text{e}^- = \text{HIO} + 2\text{H}_2\text{O}$                           | 1.14                               |                         |
| $\text{HIO}_3 + 5\text{H}^+ + 2\text{Cl}^- + 4\text{e}^- = \text{ICl}_2^- + 3\text{H}_2\text{O}$         | 1.214                              |                         |
| $2\text{IO}_3^- + 12\text{H}^+ + 10\text{e}^- = \text{I}_2(\text{c}) + 3\text{H}_2\text{O}$              | 1.195                              |                         |
| $\text{IO}_3^- + 3\text{H}_2\text{O} + 6\text{e}^- = \text{I}^- + 6\text{OH}^-$                          | 0.257                              |                         |
| $2\text{IBr}_2^- + 2\text{e}^- = \text{I}_2\text{Br}^- + 3\text{Br}^-$                                   | 0.821                              |                         |
| $2\text{IBr}_2^- + 2\text{e}^- = \text{I}_2(\text{c}) + 4\text{Br}^-$                                    | 0.874                              |                         |
| $2\text{IBr} + 2\text{e}^- = \text{I}_2\text{Br}^- + \text{Br}^-$                                        | 0.973                              |                         |
| $2\text{IBr} + 2\text{e}^- = \text{I}_2 + 2\text{Br}^-$                                                  | 1.02                               |                         |
| $2\text{ICl} + 2\text{e}^- = \text{I}_2(\text{c}) + 2\text{Cl}^-$                                        | 1.20                               |                         |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                              | Standard or formal potential | Solution composition        |
|------------------------------------------------------------------------------------------------------------|------------------------------|-----------------------------|
| $2\text{ICl}_2^- + 2e^- = \text{I}_2(\text{c}) + 4\text{Cl}^-$                                             | 1.07                         |                             |
| $2\text{ICN} + 2\text{H}^+ + 2e^- = \text{I}_2(\text{c}) + 2\text{HCN}$                                    | 0.695                        |                             |
| $2\text{ICN} + 2\text{H}^+ + 2e^- = \text{I}_2(\text{aq}) + 2\text{HCN}$                                   | 0.609                        |                             |
| $2\text{HIO} + 2\text{H}^+ + 2e^- = \text{I}_2 + 2\text{H}_2\text{O}$                                      | 1.45                         |                             |
| $\text{HIO} + \text{H}^+ + 2e^- = \text{I}^- + \text{H}_2\text{O}$                                         | 0.985                        |                             |
| $\text{I}_3^- + 2e^- = 3\text{I}^-$                                                                        | 0.536                        |                             |
| $\text{I}_2(\text{aq}) + 2e^- = 2\text{I}^-$                                                               | 0.621                        |                             |
| $\text{I}_2(\text{c}) + 2e^- = 2\text{I}^-$                                                                | 0.5355                       |                             |
| <b>Iridium</b>                                                                                             |                              |                             |
| $\text{IrBr}_6^{2-} + e^- = \text{IrBr}_6^{3-}$                                                            | 0.805                        |                             |
| $\text{IrCl}_6^{2-} + e^- = \text{IrCl}_6^{3-}$                                                            | 0.867                        |                             |
| $\text{IrI}_6^{2-} + e^- = \text{IrI}_6^{3-}$                                                              | 0.49                         |                             |
| $\text{IrO}_2 + 4\text{H}^+ + e^- = \text{Ir}^{3+} + 2\text{H}_2\text{O}$                                  | 0.223                        |                             |
| $\text{IrO}_2 + 4\text{H}^+ + 4e^- = \text{Ir} + 2\text{H}_2\text{O}$                                      | 0.935                        | 1 $\text{H}_2\text{SO}_4$   |
| $\text{Ir}^{3+} + 3e^- = \text{Ir}$                                                                        | 1.156                        |                             |
| $\text{IrCl}_6^{2-} + 4e^- = \text{Ir} + 6\text{Cl}^-$                                                     | 0.835                        |                             |
| $\text{IrCl}_6^{3-} + 3e^- = \text{Ir} + 6\text{Cl}^-$                                                     | 0.77                         |                             |
| <b>Iron</b>                                                                                                |                              |                             |
| $\text{FeO}_4^{2-} + 8\text{H}^+ + 3e^- = \text{Fe}^{3+} + 4\text{H}_2\text{O}$                            | 2.2                          |                             |
| $\text{FeO}_4^{2-} + 2\text{H}_2\text{O} + 3e^- = \text{FeO}_2^- + 4\text{OH}^-$                           | 0.55                         | 10 NaOH                     |
| $\text{Fe}^{3+} + e^- = \text{Fe}^{2+}$                                                                    | 0.771                        |                             |
|                                                                                                            | 0.70                         | 1 HCl                       |
|                                                                                                            | 0.67                         | 0.5 $\text{H}_2\text{SO}_4$ |
|                                                                                                            | 0.44                         | 0.3 $\text{H}_3\text{PO}_4$ |
| $\text{Fe}(\text{CN})_6^{3-} + e^- = \text{Fe}(\text{CN})_6^{4-}$                                          | 0.361                        |                             |
|                                                                                                            | 0.71                         | 1 HCl                       |
| $\text{Fe}(\text{EDTA})^- + e^- = \text{Fe}(\text{EDTA})^{2-}$                                             | 0.12                         | 0.1 EDTA, pH 4–6            |
| $\text{Fe}(\text{OH})_4^- + e^- = \text{Fe}(\text{OH})_3$                                                  | –0.73                        | 1 NaOH                      |
| $\text{Fe}^{2+} + 2e^- = \text{Fe}$                                                                        | –0.44                        |                             |
| $[\text{Fe}(\text{CO})_4]_3 + 6e^- = 3\text{Fe}(\text{CO})_2^-$                                            | –0.70                        |                             |
| <b>Lanthanum</b>                                                                                           |                              |                             |
| $\text{La}^{3+} + 3e^- = \text{La}$                                                                        | –2.38                        |                             |
| <b>Lawrencium</b>                                                                                          |                              |                             |
| $\text{Lr}^{3+} + 3e^- = \text{Lr}$                                                                        | –2.0                         |                             |
| <b>Lead</b>                                                                                                |                              |                             |
| $\text{Pb}^{4+} + 2e^- = \text{Pb}^{2+}$                                                                   | 1.65                         |                             |
| $\text{PbO}_2(\text{alpha}) + \text{SO}_4^{2-} + 4\text{H}^+ + 2e^- = \text{PbSO}_4 + 2\text{H}_2\text{O}$ | 1.690                        |                             |
| $\text{PbO}_2 + 4\text{H}^+ + 2e^- = \text{Pb}^{2+} + 2\text{H}_2\text{O}$                                 | 1.46                         |                             |
| $\text{PbO}_2 + 2\text{H}^+ + 2e^- = \text{PbO} + \text{H}_2\text{O}$                                      | 0.28                         |                             |
| $\text{PbO}_2^- + \text{H}_2\text{O} + 2e^- = \text{HPbO}_2^- + 3\text{OH}^-$                              | 0.3                          | 2 NaOH                      |
| $\text{Pb}^{2+} + 2e^- = \text{Pb}$                                                                        | –0.126                       |                             |
| $\text{HPbO}_2^- + \text{H}_2\text{O} + 2e^- = \text{Pb} + 3\text{OH}^-$                                   | –0.54                        |                             |
| $\text{PbHPO}_4 + 2e^- = \text{Pb} + \text{HPO}_4^{2-}$                                                    | –0.465                       |                             |
| $\text{PbSO}_4 + 2e^- = \text{Pb} + \text{SO}_4^{2-}$                                                      | –0.356                       |                             |
| $\text{PbF}_2 + 2e^- = \text{Pb} + 2\text{F}^-$                                                            | –0.344                       |                             |
| $\text{PbCl}_2 + 2e^- = \text{Pb} + 2\text{Cl}^-$                                                          | –0.268                       |                             |
| $\text{PbBr}_2 + 2e^- = \text{Pb} + 2\text{Br}^-$                                                          | –0.280                       |                             |
| $\text{PbI}_2 + 2e^- = \text{Pb} + 2\text{I}^-$                                                            | –0.365                       |                             |
| $\text{Pb} + 2\text{H}^+ + 2e^- = \text{PbH}_2$                                                            | –1.507                       |                             |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                                                          | Standard<br>or formal<br>potential | Solution<br>composition                   |
|----------------------------------------------------------------------------------------------------------------------------------------|------------------------------------|-------------------------------------------|
| <b>Lithium</b>                                                                                                                         |                                    |                                           |
| $\text{Li}^+ + e^- = \text{Li}$                                                                                                        | -3.040                             |                                           |
| $\text{Li}^+ + \text{Hg} + e^- = \text{Li(Hg)}$                                                                                        | -2.00                              |                                           |
| <b>Lutetium</b>                                                                                                                        |                                    |                                           |
| $\text{Lu}^{3+} + 3e^- = \text{Lu}$                                                                                                    | -2.30                              |                                           |
| <b>Magnesium</b>                                                                                                                       |                                    |                                           |
| $\text{Mg}^{2+} + 2e^- = \text{Mg}$                                                                                                    | -2.356                             |                                           |
| $\text{Mg(OH)}_2 + 2e^- = \text{Mg} + 2\text{OH}^-$                                                                                    | -2.687                             |                                           |
| <b>Manganese</b>                                                                                                                       |                                    |                                           |
| $\text{MnO}_4^- + e^- = \text{MnO}_4^{2-}$                                                                                             | 0.56                               |                                           |
| $\text{MnO}_4^- + 4\text{H}^+ + 3e^- = \text{MnO}_2(\text{beta}) + 2\text{H}_2\text{O}$                                                | 1.70                               |                                           |
| $\text{MnO}_4^- + 2\text{H}_2\text{O} + 3e^- = \text{MnO}_2 + 4\text{OH}^-$                                                            | 0.60                               |                                           |
| $\text{MnO}_4^- + 8\text{H}^+ + 5e^- = \text{Mn}^{2+} + 4\text{H}_2\text{O}$                                                           | 1.51                               |                                           |
| $\text{MnO}_4^{2-} + e^- = \text{MnO}_4^{3-}$                                                                                          | 0.27                               |                                           |
| $\text{MnO}_4^{2-} + 2\text{H}_2\text{O} + 2e^- = \text{MnO}_2 + 4\text{OH}^-$                                                         | 0.62                               |                                           |
| $\text{MnO}_3^- + 2\text{H}_2\text{O} + e^- = \text{MnO}_2 + 4\text{OH}^-$                                                             | 0.96                               |                                           |
| $\text{MnO}_2 + 4\text{H}^+ + e^- = \text{Mn}^{3+} + 2\text{H}_2\text{O}$                                                              | 0.95                               |                                           |
| $\text{MnO}_2(\text{beta}) + 4\text{H}^+ + 2e^- = \text{Mn}^{2+} + 2\text{H}_2\text{O}$                                                | 1.23                               |                                           |
| $\text{Mn}^{3+} + e^- = \text{Mn}^{2+}$                                                                                                | 1.5                                |                                           |
| $\text{Mn(H}_2\text{P}_2\text{O}_7)_3^- + 2\text{H}^+ + e^- = \text{Mn(H}_2\text{P}_2\text{O}_7)_2^- + \text{H}_4\text{P}_2\text{O}_7$ | 1.15                               | 0.4 $\text{H}_2\text{P}_2\text{O}_7^{2-}$ |
| $\text{Mn(CN)}_6^{3-} + e^- = \text{Mn(CN)}_6^{4-}$                                                                                    | -0.24                              | 1.5 NaCN                                  |
| $\text{Mn}^{2+} + 2e^- = \text{Mn}$                                                                                                    | -1.17                              |                                           |
| <b>Mendelevium</b>                                                                                                                     |                                    |                                           |
| $\text{Md}^{3+} + 3e^- = \text{Md}$                                                                                                    | -1.7                               |                                           |
| $\text{Md}^{3+} + e^- = \text{Md}^{2+}$                                                                                                | -0.15                              |                                           |
| $\text{Md}^{2+} + 2e^- = \text{Md}$                                                                                                    | -2.4                               |                                           |
| <b>Mercury</b>                                                                                                                         |                                    |                                           |
| $2\text{Hg}^{2+} + 2e^- = \text{Hg}_2^{2+}$                                                                                            | 0.911                              |                                           |
| $2\text{HgCl}_2 + 2e^- = \text{Hg}_2\text{Cl}_2 + 2\text{Cl}^-$                                                                        | 0.63                               |                                           |
| $\text{Hg}^{2+} + 2e^- = \text{Hg(lq)}$                                                                                                | 0.8535                             |                                           |
| $\text{HgO(c,red)} + 2\text{H}^+ + 2e^- = \text{Hg} + \text{H}_2\text{O}$                                                              | 0.926                              |                                           |
| $\text{Hg}_2^{2+} + 2e^- = 2\text{Hg}$                                                                                                 | 0.7960                             |                                           |
| $\text{Hg}_2\text{F}_2 + 2e^- = 2\text{Hg} + 2\text{F}^-$                                                                              | 0.656                              |                                           |
| $\text{Hg}_2\text{Cl}_2 + 2e^- = 2\text{Hg} + 2\text{Cl}^-$                                                                            | 0.2682                             |                                           |
| $\text{Hg}_2\text{Br}_2 + 2e^- = 2\text{Hg} + 2\text{Br}^-$                                                                            | 0.1392                             |                                           |
| $\text{Hg}_2\text{I}_2 + 2e^- = 2\text{Hg} + 2\text{I}^-$                                                                              | -0.0405                            |                                           |
| $\text{Hg}_2\text{SO}_4 + 2e^- = 2\text{Hg} + \text{SO}_4^{2-}$                                                                        | 0.614                              |                                           |
| <b>Molybdenum</b>                                                                                                                      |                                    |                                           |
| $\text{MoO}_4^{2-} + 4\text{H}_2\text{O} + 6e^- = \text{Mo} + 8\text{OH}^-$                                                            | -0.913                             |                                           |
| $\text{H}_2\text{MoO}_4 + 6\text{H}^+ + 6e^- = \text{Mo} + 4\text{H}_2\text{O}$                                                        | 0.114                              |                                           |
| $\text{H}_2\text{MoO}_4 + 2\text{H}^+ + 2e^- = \text{MoO}_2 + 2\text{H}_2\text{O}$                                                     | 0.646                              |                                           |
| $\text{MoO}_2 + 4\text{H}^+ + 4e^- = \text{Mo} + 2\text{H}_2\text{O}$                                                                  | -0.152                             |                                           |
| $\text{H}_2\text{MoO}_4 + 6\text{H}^+ + 3e^- = \text{Mo}^{3+} + 4\text{H}_2\text{O}$                                                   | 0.428                              |                                           |
| $\text{Mo(CN)}_6^{3-} + e^- = \text{Mo(CN)}_6^{4-}$                                                                                    | 0.725                              |                                           |
| $\text{Mo}^{3+} + 3e^- = \text{Mo}$                                                                                                    | -0.2                               |                                           |
| <b>Neodymium</b>                                                                                                                       |                                    |                                           |
| $\text{Nd}^{3+} + 3e^- = \text{Nd}$                                                                                                    | -2.32                              |                                           |
| $\text{Nd}^{3+} + e^- = \text{Nd}^{2+}$                                                                                                | -2.6                               |                                           |
| $\text{Nd}^{2+} + 2e^- = \text{Nd}$                                                                                                    | -2.2                               |                                           |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                                 | Standard or formal potential | Solution composition |
|---------------------------------------------------------------------------------------------------------------|------------------------------|----------------------|
| <b>Neptunium</b>                                                                                              |                              |                      |
| $\text{NpO}_3^+ + 2\text{H}^+ + e^- = \text{NpO}_2^{2+} + \text{H}_2\text{O}$                                 | 2.04                         |                      |
| $\text{NpO}_2^{2+} + e^- = \text{NpO}_2^+$                                                                    | 1.34                         |                      |
| $\text{NpO}_2^+ + 4\text{H}^+ + 2e^- = \text{Np}^{4+} + 2\text{H}_2\text{O}$                                  | 0.95                         |                      |
| $\text{Np}^{4+} + e^- = \text{Np}^{3+}$                                                                       | 0.18                         |                      |
| $\text{Np}^{4+} + 4e^- = \text{Np}$                                                                           | -1.30                        |                      |
| $\text{Np}^{3+} + 3e^- = \text{Np}$                                                                           | -1.79                        |                      |
| <b>Nickel</b>                                                                                                 |                              |                      |
| $\text{NiO}_2^- + 4\text{H}^+ + 2e^- = \text{NiO}_2 + 2\text{H}_2\text{O}$                                    | 1.8                          |                      |
| $\text{NiO}_2 + 4\text{H}^+ + 2e^- = \text{Ni}^{2+} + 2\text{H}_2\text{O}$                                    | 1.593                        |                      |
| $\text{NiO}_2 + 2\text{H}_2\text{O} + 2e^- = \text{Ni}(\text{OH})_2 + 2\text{OH}^-$                           | 0.490                        |                      |
| $\text{Ni}(\text{CN})_4^{2-} + e^- = \text{Ni}(\text{CN})_3^- + \text{CN}^-$                                  | -0.401                       |                      |
| $\text{Ni}^{2+} + 2e^- = \text{Ni}$                                                                           | -0.257                       |                      |
| $\text{Ni}(\text{OH})_2 + 2e^- = \text{Ni} + 2\text{OH}^-$                                                    | -0.72                        |                      |
| $\text{Ni}(\text{NH}_3)_6^{2+} + 2e^- = \text{Ni} + 6\text{NH}_3$                                             | -0.49                        |                      |
| <b>Niobium</b>                                                                                                |                              |                      |
| $\text{Nb}_2\text{O}_5 + 10\text{H}^+ + 4e^- = 2\text{Nb}^{3+} + 5\text{H}_2\text{O}$                         | -0.1                         |                      |
| $\text{Nb}_2\text{O}_5 + 10\text{H}^+ + 10e^- = 2\text{Nb} + 5\text{H}_2\text{O}$                             | -0.65                        |                      |
| $\text{Nb}^{3+} + 3e^- = \text{Nb}$                                                                           | -1.1                         |                      |
| <b>Nitrogen</b>                                                                                               |                              |                      |
| $2\text{NO}_3^- + 4\text{H}^+ + 2e^- = \text{N}_2\text{O}_4 + 2\text{H}_2\text{O}$                            | 0.803                        |                      |
| $\text{NO}_3^- + 3\text{H}^+ + 2e^- = \text{HNO}_2 + \text{H}_2\text{O}$                                      | 0.94                         |                      |
| $\text{N}_2\text{O}_4 + 2\text{H}^+ + 2e^- = 2\text{HNO}_2$                                                   | 1.07                         |                      |
| $\text{HNO}_2 + \text{H}^+ + e^- = \text{NO} + \text{H}_2\text{O}$                                            | 0.996                        |                      |
| $2\text{HNO}_2 + 4\text{H}^+ + 4e^- = \text{N}_2\text{O}(\text{g}) + 3\text{H}_2\text{O}$                     | 1.297                        |                      |
| $2\text{HNO}_2 + 4\text{H}^+ + 4e^- = \text{H}_2\text{N}_2\text{O}_2 + 2\text{H}_2\text{O}$                   | 0.86                         |                      |
| $2\text{NO} + 2\text{H}^+ + 2e^- = \text{H}_2\text{N}_2\text{O}_2$                                            | 0.71                         |                      |
| $2\text{NO} + 2\text{H}^+ + 2e^- = \text{N}_2\text{O} + \text{H}_2\text{O}$                                   | 1.59                         |                      |
| $\text{H}_2\text{N}_2\text{O}_2 + 6\text{H}^+ + 4e^- = 2\text{HONH}_3^+$                                      | 0.496                        |                      |
| $\text{N}_2\text{O} + 2\text{H}^+ + 2e^- = \text{N}_2 + \text{H}_2\text{O}$                                   | 1.77                         |                      |
| $\text{N}_2\text{O} + 6\text{H}^+ + \text{H}_2\text{O} + 4e^- = 2\text{HONH}_3^+$                             | -0.05                        |                      |
| $\text{N}_2 + 2\text{H}_2\text{O} + 4\text{H}^+ + 2e^- = 2\text{HONH}_3^+$                                    | -1.87                        |                      |
| $\text{N}_2 + 5\text{H}^+ + 4e^- = \text{N}_2\text{H}_5^+$                                                    | -0.23                        |                      |
| $\text{HONH}_3^+ + 2\text{H}^+ + 2e^- = \text{NH}_4^+ + \text{H}_2\text{O}$                                   | 1.35                         |                      |
| $2\text{HONH}_3^+ + \text{H}^+ + 2e^- = \text{N}_2\text{H}_5^+ + 2\text{H}_2\text{O}$                         | 1.41                         |                      |
| $\text{N}_2\text{H}_5^+ + 3\text{H}^+ + 2e^- = 2\text{NH}_4^+$                                                | 1.275                        |                      |
| $3\text{N}_2 + 2\text{H}^+ + 2e^- = 2\text{HN}_3$                                                             | -3.40                        |                      |
| <b>Nobelium</b>                                                                                               |                              |                      |
| $\text{No}^{3+} + 3e^- = \text{No}$                                                                           | -1.2                         |                      |
| $\text{No}^{3+} + e^- = \text{No}^{2+}$                                                                       | 1.4                          |                      |
| $\text{No}^{2+} + 2e^- = \text{No}$                                                                           | -2.5                         |                      |
| <b>Osmium</b>                                                                                                 |                              |                      |
| $\text{OsO}_4(\text{aq}) + 4\text{H}^+ + 4e^- = \text{OsO}_2 \cdot 2\text{H}_2\text{O} + 2\text{H}_2\text{O}$ | 0.964                        |                      |
| $\text{OsO}_4(\text{c, yellow}) + 8\text{H}^+ + 8e^- = \text{Os} + 4\text{H}_2\text{O}$                       | 0.85                         |                      |
| $\text{OsO}_2 + 4\text{H}^+ + 4e^- = \text{Os} + 2\text{H}_2\text{O}$                                         | 0.687                        |                      |
| $\text{OsCl}_6^{2-} + e^- = \text{OsCl}_6^{3-}$                                                               | 0.45                         |                      |
| $\text{OsBr}_6^{2-} + e^- = \text{OsBr}_6^{3-}$                                                               | 0.35                         |                      |
| <b>Oxygen</b>                                                                                                 |                              |                      |
| $\text{O}_3 + 2\text{H}^+ + 2e^- = \text{O}_2 + \text{H}_2\text{O}$                                           | 2.075                        |                      |
| $\text{O}_3 + \text{H}_2\text{O} + 2e^- = \text{O}_2 + 2\text{OH}^-$                                          | 1.240                        | 1 NaOH               |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                               | Standard<br>or formal<br>potential | Solution<br>composition                  |
|-------------------------------------------------------------------------------------------------------------|------------------------------------|------------------------------------------|
| $\text{O}_2 + 4\text{H}^+ + 4\text{e}^- = 2\text{H}_2\text{O}$                                              | 1.229                              | 1 NaOH                                   |
| $\text{O}_2 + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{O}$                                               | 0.695                              |                                          |
| $\text{O}_2 + \text{H}_2\text{O} + 2\text{e}^- = \text{HO}_2^- + \text{OH}^-$                               | -0.076                             |                                          |
| $\text{H}_2\text{O}_2 + 2\text{H}^+ + 2\text{e}^- = 2\text{H}_2\text{O}$                                    | 1.763                              |                                          |
| $\text{HO}_2^- + \text{H}_2\text{O} + 2\text{e}^- = 3\text{OH}^-$                                           | 0.867                              |                                          |
| $\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- = 4\text{OH}^-$                                             | 0.401                              |                                          |
| <b>Palladium</b>                                                                                            |                                    |                                          |
| $\text{PdO}_3 + 2\text{H}^+ + 2\text{e}^- = \text{PdO}_2 + \text{H}_2\text{O}$                              | 2.030                              | 1 HCl                                    |
| $\text{PdCl}_6^{2-} + 2\text{e}^- = \text{PdCl}_4^{2-} + 2\text{Cl}^-$                                      | 1.470                              |                                          |
| $\text{PdBr}_6^{2-} + 2\text{e}^- = \text{PdBr}_4^{2-} + 2\text{Br}^-$                                      | 0.99                               |                                          |
| $\text{PdI}_6^{2-} + 2\text{e}^- = \text{PdI}_4^{2-} + 2\text{I}^-$                                         | 0.48                               |                                          |
| $\text{Pd}^{2+} + 2\text{e}^- = \text{Pd}$                                                                  | 0.915                              |                                          |
| $\text{PdCl}_4^{2-} + 2\text{e}^- = \text{Pd} + 4\text{Cl}^-$                                               | 0.62                               |                                          |
| $\text{PdBr}_4^{2-} + 2\text{e}^- = \text{Pd} + 4\text{Br}^-$                                               | 0.49                               | 1 NH <sub>3</sub>                        |
| $\text{Pd}(\text{NH}_3)_4^{2+} + 2\text{e}^- = \text{Pd} + 4\text{NH}_3$                                    | 0.0                                |                                          |
| $\text{Pd}(\text{CN})_4^{2-} + 2\text{e}^- = \text{Pd} + 4\text{CN}^-$                                      | -1.35                              | 1 KCN                                    |
| <b>Phosphorus</b>                                                                                           |                                    |                                          |
| $\text{H}_3\text{PO}_4 + 2\text{H}^+ + 2\text{e}^- = \text{H}_3\text{PO}_3 + \text{H}_2\text{O}$            | -0.276                             |                                          |
| $2\text{H}_3\text{PO}_4 + 2\text{H}^+ + 2\text{e}^- = \text{H}_4\text{P}_2\text{O}_6 + 2\text{H}_2\text{O}$ | -0.933                             |                                          |
| $\text{H}_4\text{P}_2\text{O}_6 + 2\text{H}^+ + 2\text{e}^- = 2\text{H}_3\text{PO}_3$                       | 0.380                              |                                          |
| $\text{H}_3\text{PO}_3 + 2\text{H}^+ + 2\text{e}^- = \text{HPH}_2\text{O}_2 + \text{H}_2\text{O}$           | -0.499                             |                                          |
| $\text{HPH}_2\text{O}_2 + \text{H}^+ + \text{e}^- = \text{P} + 2\text{H}_2\text{O}$                         | -0.365                             |                                          |
| $\text{H}_3\text{PO}_3 + 3\text{H}^+ + 3\text{e}^- = \text{P} + 3\text{H}_2\text{O}$                        | -0.502                             |                                          |
| $2\text{P}(\text{white}) + 4\text{H}^+ + 4\text{e}^- = \text{P}_2\text{H}_4$                                | -0.100                             |                                          |
| $\text{P}_2\text{H}_4 + 2\text{H}^+ + 2\text{e}^- = 2\text{PH}_3$                                           | -0.006                             |                                          |
| $\text{P}(\text{white}) + 3\text{H}^+ + 3\text{e}^- = \text{PH}_3$                                          | -0.063                             |                                          |
| <b>Platinum</b>                                                                                             |                                    |                                          |
| $\text{PtO}_3 + 2\text{H}^+ + 2\text{e}^- = \text{PtO}_2 + \text{H}_2\text{O}$                              | 2.0                                | 1 KBr                                    |
| $\text{PtO}_2 + 2\text{H}^+ + 2\text{e}^- = \text{PtO} + \text{H}_2\text{O}$                                | 1.045                              |                                          |
| $\text{PtCl}_6^{2-} + 2\text{e}^- = \text{PtCl}_4^{2-} + 2\text{Cl}^-$                                      | 0.726                              |                                          |
| $\text{PtBr}_6^{2-} + 2\text{e}^- = \text{PtBr}_4^{2-} + 2\text{Br}^-$                                      | 0.613                              |                                          |
| $\text{PtI}_6^{2-} + 2\text{e}^- = \text{PtI}_4^{2-} + 2\text{I}^-$                                         | 0.321                              |                                          |
| $\text{Pt}^{2+} + 2\text{e}^- = \text{Pt}$                                                                  | 1.188                              |                                          |
| $\text{PtCl}_4^{2-} + 2\text{e}^- = \text{Pt} + 4\text{Cl}^-$                                               | 0.758                              | 1 KI                                     |
| $\text{PtBr}_4^{2-} + 2\text{e}^- = \text{Pt} + 4\text{Br}^-$                                               | 0.698                              |                                          |
| <b>Plutonium</b>                                                                                            |                                    |                                          |
| $\text{PuO}_2^{2+} + \text{e}^- = \text{PuO}_2^+$                                                           | 1.02                               | 1 H <sub>3</sub> PO <sub>4</sub><br>1 HF |
| $\text{PuO}_2^{2+} + 4\text{H}^+ + 2\text{e}^- = \text{Pu}^{4+} + 2\text{H}_2\text{O}$                      | 1.04                               |                                          |
| $\text{Pu}^{4+} + \text{e}^- = \text{Pu}^{3+}$                                                              | 1.01                               |                                          |
|                                                                                                             | 0.80                               |                                          |
|                                                                                                             | 0.50                               |                                          |
| $\text{Pu}^{4+} + 4\text{e}^- = \text{Pu}$                                                                  | -1.25                              |                                          |
| $\text{Pu}^{3+} + 3\text{e}^- = \text{Pu}$                                                                  | -2.00                              |                                          |
| <b>Polonium</b>                                                                                             |                                    |                                          |
| $\text{PoO}_2 + 4\text{H}^+ + 2\text{e}^- = \text{Po}^{2+} + 2\text{H}_2\text{O}$                           | 1.1                                | ca. -1.0                                 |
| $\text{Po}^{4+} + 4\text{e}^- = \text{Po}$                                                                  | 0.73                               |                                          |
| $\text{Po}^{2+} + 2\text{e}^- = \text{Po}$                                                                  | 0.37                               |                                          |
| $\text{Po} + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{Po}$                                               |                                    |                                          |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                         | Standard or formal potential | Solution composition |
|-------------------------------------------------------|------------------------------|----------------------|
| <b>Potassium</b>                                      |                              |                      |
| $K^+ + e^- = K$                                       | -2.924                       |                      |
| $K^+ + Hg + e^- = K(Hg)$                              | ca. -1.9                     |                      |
| <b>Praseodymium</b>                                   |                              |                      |
| $Pr^{4+} + e^- = Pr^{3+}$                             | 3.2                          |                      |
| $Pr^{3+} + e^- = Pr$                                  | -2.35                        |                      |
| <b>Promethium</b>                                     |                              |                      |
| $Pm^{3+} + 3e^- = Pm$                                 | -2.42                        |                      |
| <b>Protoactinium</b>                                  |                              |                      |
| $PaOOH^{2+} + 3H^+ + e^- = Pa^{4+} + 2H_2O$           | -0.10                        |                      |
| $PaOOH^{2+} + 3H^+ + 5e^- = Pa + 2H_2O$               | -1.19                        |                      |
| $Pa^{4+} + 4e^- = Pa$                                 | -1.46                        |                      |
| <b>Radium</b>                                         |                              |                      |
| $Ra^{2+} + 2e^- = Ra$                                 | -2.916                       |                      |
| <b>Rhenium</b>                                        |                              |                      |
| $ReO_4^- + 2H^+ + e^- = ReO_3 + H_2O$                 | 0.768                        |                      |
| $ReO_4^- + 4H^+ + 3e^- = ReO_2 + 2H_2O$               | 0.51                         |                      |
| $ReO_4^- + 2H_2O + 3e^- = ReO_2 + 4OH^-$              | -0.594                       |                      |
| $ReO_4^- + 6Cl^- + 8H^+ + 3e^- = ReCl_6^{3-} + 4H_2O$ | 0.12                         |                      |
| $2ReO_4^- + 10H^+ + 8e^- = Re_2O_3 + 5H_2O$           | -0.808                       |                      |
| $ReO_3 + 2H^+ + 2e^- = ReO_2 + H_2O$                  | 0.63                         |                      |
| $ReO_2 + 4H^+ + 4e^- = Re + 2H_2O$                    | 0.22                         |                      |
| $ReCl_6^{3-} + 4e^- = Re + 6Cl^-$                     | 0.51                         |                      |
| $Re + e^- = Re^-$                                     | -0.10                        |                      |
| <b>Rhodium</b>                                        |                              |                      |
| $RhO_2 + 4H^+ + e^- = Rh^{3+} + 2H_2O$                | 1.881                        |                      |
| $Rh^{3+} + 3e^- = Rh$                                 | 0.76                         |                      |
| $RhCl_3 + 3e^- = Rh + 6Cl^-$                          | 0.5                          |                      |
| <b>Rubidium</b>                                       |                              |                      |
| $Rb^+ + e^- = Rb$                                     | -2.924                       |                      |
| $Rb^+ + Hg + e^- = Rb(Hg)$                            | -1.81                        |                      |
| <b>Ruthenium</b>                                      |                              |                      |
| $RuO_4 + e^- = RuO_4^-$                               | 0.89                         |                      |
| $RuO_4 + 4H^+ + 4e^- = RuO_2 + 2H_2O$                 | 1.4                          |                      |
| $RuO_4 + 8H^+ + 8e^- = Ru + 4H_2O$                    | 1.04                         |                      |
| $RuO_4^- + e^- = RuO_4^{2-}$                          | 0.593                        |                      |
| $RuO_4^{2-} + 4H^+ + 2e^- = RuO_2 + 2H_2O$            | 2.0                          |                      |
| $RuO_2 + 4H^+ + 4e^- = Ru + 2H_2O$                    | 0.68                         |                      |
| $Ru(H_2O)_6^{3+} + e^- = Ru(H_2O)_6^{2+}$             | 0.249                        |                      |
| $Ru(NH_3)_6^{3+} + e^- = Ru(NH_3)_6^{2+}$             | 0.10                         |                      |
| $Ru(CN)_6^{3-} + e^- = Ru(CN)_6^{4-}$                 | 0.86                         |                      |
| $Ru^{3+} + e^- = Ru^{2+}$                             | 0.249                        |                      |
| <b>Samarium</b>                                       |                              |                      |
| $Sm^{3+} + 3e^- = Sm$                                 | -2.30                        |                      |
| $Sm^{3+} + e^- = Sm^{2+}$                             | -1.55                        |                      |
| $Sm^{2+} + 2e^- = Sm$                                 | -2.67                        |                      |
| <b>Scandium</b>                                       |                              |                      |
| $Sc^{3+} + 3e^- = Sc$                                 | -2.03                        |                      |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                          | Standard<br>or formal<br>potential | Solution<br>composition |
|--------------------------------------------------------------------------------------------------------|------------------------------------|-------------------------|
| <b>Selenium</b>                                                                                        |                                    |                         |
| $\text{SeO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- = \text{H}_2\text{SeO}_3 + \text{H}_2\text{O}$          | 1.151                              | 1 NaOH                  |
| $\text{H}_2\text{SeO}_3 + 4\text{H}^+ + 4\text{e}^- = \text{Se} + 3\text{H}_2\text{O}$                 | 0.74                               |                         |
| $\text{Se}(\text{c}) + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{Se}(\text{aq})$                     | -0.115                             |                         |
| $\text{Se} + \text{H}^+ + 2\text{e}^- = \text{HSe}^-$                                                  | -0.227                             |                         |
| $\text{Se} + 2\text{e}^- = \text{Se}^{2-}$                                                             | -0.670                             |                         |
|                                                                                                        |                                    |                         |
| <b>Silicon</b>                                                                                         |                                    |                         |
| $\text{SiO}_2(\text{quartz}) + 4\text{H}^+ + 4\text{e}^- = \text{Si} + 2\text{H}_2\text{O}$            | -0.909                             | 1 NaOH                  |
| $\text{SiO}_2 + 2\text{H}^+ + 2\text{e}^- = \text{SiO} + \text{H}_2\text{O}$                           | -0.967                             |                         |
| $\text{SiO}_2 + 8\text{H}^+ + 8\text{e}^- = \text{SiH}_4 + 2\text{H}_2\text{O}$                        | -0.516                             |                         |
| $\text{SiF}_6^{2-} + 4\text{e}^- = \text{Si} + 6\text{F}^-$                                            | -1.37                              |                         |
| $\text{SiO} + 2\text{H}^+ + 2\text{e}^- = \text{Si} + \text{H}_2\text{O}$                              | -0.808                             |                         |
| $\text{Si} + 4\text{H}^+ + 4\text{e}^- = \text{SiH}_4(\text{g})$                                       | -0.143                             |                         |
|                                                                                                        |                                    |                         |
| <b>Silver</b>                                                                                          |                                    |                         |
| $\text{AgO}^+ + 2\text{H}^+ + \text{e}^- = \text{Ag}^{2+} + \text{H}_2\text{O}$                        | 1.360                              | 1 NaOH                  |
| $\text{Ag}_2\text{O}_3 + 2\text{H}^+ + 2\text{e}^- = 2\text{AgO} + \text{H}_2\text{O}$                 | 1.569                              |                         |
| $\text{Ag}_2\text{O}_3 + \text{H}_2\text{O} + 2\text{e}^- = 2\text{AgO} + 2\text{OH}^-$                | 0.739                              |                         |
| $\text{Ag}_2\text{O}_3 + 6\text{H}^+ + 4\text{e}^- = 2\text{Ag}^+ + 3\text{H}_2\text{O}$               | 1.670                              |                         |
| $\text{Ag}^{2+} + \text{e}^- = \text{Ag}^+$                                                            | 1.980                              |                         |
| $\text{AgO} + 2\text{H}^+ + \text{e}^- = \text{Ag}^+ + \text{H}_2\text{O}$                             | 1.772                              |                         |
| $\text{Ag}^+ + \text{e}^- = \text{Ag}$                                                                 | 0.7991                             |                         |
| $\text{Ag}_2\text{SO}_4 + 2\text{e}^- = 2\text{Ag} + \text{SO}_4^{2-}$                                 | 0.653                              |                         |
| $\text{Ag}_2\text{C}_2\text{O}_4 + 2\text{e}^- = 2\text{Ag} + \text{C}_2\text{O}_4^{2-}$               | 0.47                               |                         |
| $\text{Ag}_2\text{CrO}_4 + 2\text{e}^- = 2\text{Ag} + \text{CrO}_4^{2-}$                               | 0.447                              |                         |
| $\text{Ag}(\text{NH}_3)_2^+ + \text{e}^- = \text{Ag} + 2\text{NH}_3$                                   | 0.373                              |                         |
| $\text{AgCl} + \text{e}^- = \text{Ag} + \text{Cl}^-$                                                   | 0.2223                             |                         |
| $\text{AgBr} + \text{e}^- = \text{Ag} + \text{Br}^-$                                                   | 0.071                              |                         |
| $\text{AgCN} + \text{e}^- = \text{Ag} + \text{CN}^-$                                                   | -0.017                             |                         |
| $\text{AgI} + \text{e}^- = \text{Ag} + \text{I}^-$                                                     | -0.152                             |                         |
| $\text{Ag}(\text{CN}) + \text{e}^- = \text{Ag} + 2\text{CN}^-$                                         | -0.31                              |                         |
| $\text{AgSCN} + \text{e}^- = \text{Ag} + \text{SCN}^-$                                                 | 0.09                               |                         |
| $\text{Ag}_2\text{S} + 2\text{e}^- = 2\text{Ag} + \text{S}^{2-}$                                       | -0.71                              |                         |
|                                                                                                        |                                    |                         |
| <b>Sodium</b>                                                                                          |                                    |                         |
| $\text{Na}^+ + \text{e}^- = \text{Na}$                                                                 | -2.713                             | 1 NaOH                  |
| $\text{Na}^+ + \text{Hg} + \text{e}^- = \text{Na}(\text{Hg})$                                          | -1.84                              |                         |
|                                                                                                        |                                    |                         |
| <b>Strontium</b>                                                                                       |                                    |                         |
| $\text{SrO}_2 + 4\text{H}^+ + 2\text{e}^- = \text{Sr}^{2+}$                                            | 2.33                               | 1 NaOH                  |
| $\text{Sr}^{2+} + 2\text{e}^- = \text{Sr}$                                                             | -2.89                              |                         |
|                                                                                                        |                                    |                         |
| <b>Sulfur</b>                                                                                          |                                    |                         |
| $\text{S}_2\text{O}_8^{2-} + 2\text{e}^- = 2\text{SO}_4^{2-}$                                          | 1.96                               | 1 NaOH                  |
| $\text{S}_2\text{O}_8^{2-} + 2\text{H}^+ + 2\text{e}^- = 2\text{HSO}_4^-$                              | 2.08                               |                         |
| $2\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- = \text{S}_2\text{O}_6^{2-} + 2\text{H}_2\text{O}$      | -0.25                              |                         |
| $\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- = \text{SO}_2(\text{aq}) + \text{H}_2\text{O}$           | 0.158                              |                         |
| $\text{SO}_4^{2-} + \text{H}_2\text{O} + 2\text{e}^- = \text{SO}_3^{2-} + 2\text{OH}^-$                | -0.936                             |                         |
| $\text{S}_2\text{O}_6^{2-} + 4\text{H}^+ + 2\text{e}^- = 2\text{H}_2\text{SO}_3$                       | 0.569                              |                         |
| $\text{S}_2\text{O}_6^{2-} + 2\text{e}^- = 2\text{SO}_3^{2-}$                                          | 0.037                              |                         |
| $2\text{HSO}_3^- + 2\text{H}^+ + 2\text{e}^- = \text{S}_2\text{O}_4^{2-} + 2\text{H}_2\text{O}$        | 0.099                              |                         |
| $2\text{SO}_3^{2-} + 2\text{H}_2\text{O} + 2\text{e}^- = \text{S}_2\text{O}_4^{2-} + 4\text{OH}^-$     | -1.13                              |                         |
| $4\text{H}_2\text{SO}_3 + 4\text{H}^+ + 6\text{e}^- = \text{S}_4\text{O}_6^{2-} + 6\text{H}_2\text{O}$ | 0.507                              |                         |
|                                                                                                        |                                    |                         |
|                                                                                                        |                                    |                         |
|                                                                                                        |                                    |                         |
|                                                                                                        |                                    |                         |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                                          | Standard<br>or formal<br>potential | Solution<br>composition |  |
|--------------------------------------------------------------------------------------------------------|------------------------------------|-------------------------|--|
| $4\text{HSO}_3^- + 8\text{H}^+ + 6\text{e}^- = \text{S}_4\text{O}_6^{2-} + 6\text{H}_2\text{O}$        | 0.577                              | 1 NaOH<br>1 NaOH        |  |
| $2\text{SO}_2(\text{aq}) + 2\text{H}^+ + 4\text{e}^- = \text{S}_2\text{O}_3^{2-} + \text{H}_2\text{O}$ | 0.400                              |                         |  |
| $2\text{SO}_3^{2-} + 3\text{H}_2\text{O} + 4\text{e}^- = \text{S}_2\text{O}_3^{2-} + 6\text{OH}^-$     | −0.576                             |                         |  |
| $\text{SO}_3^{2-} + 3\text{H}_2\text{O} + 4\text{e}^- = \text{S} + 6\text{OH}^-$                       | −0.59                              |                         |  |
| $\text{S}_4\text{O}_6^{2-} + 2\text{e}^- = 2\text{S}_2\text{O}_3^{2-}$                                 | 0.080                              |                         |  |
| $\text{S}_2\text{O}_3^{2-} + 6\text{H}^+ + 4\text{e}^- = 2\text{S} + 3\text{H}_2\text{O}$              | 0.5                                |                         |  |
| $\text{SF}_4(\text{g}) + 4\text{e}^- = \text{S} + 4\text{F}^-$                                         | 0.97                               |                         |  |
| $\text{S}_2\text{Cl}_2(\text{g}) + 2\text{e}^- = 2\text{S} + 2\text{Cl}^-$                             | 1.19                               |                         |  |
| $\text{S} + \text{H}^+ + 2\text{e}^- = \text{HS}^-$                                                    | 0.287                              |                         |  |
| $\text{S} + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{S}(\text{aq})$                                 | 0.144                              |                         |  |
| $\text{S} + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{S}(\text{g})$                                  | 0.174                              |                         |  |
| $\text{S} + 2\text{e}^- = \text{S}^{2-}$                                                               | −0.407                             |                         |  |
| <b>Tantalum</b>                                                                                        |                                    |                         |  |
| $\text{Ta}_2\text{O}_5 + 10\text{H}^+ + 10\text{e}^- = 2\text{Ta} + 5\text{H}_2\text{O}$               | −0.81                              |                         |  |
| $\text{TaF}_6^{3-} + 5\text{e}^- = \text{Ta} + 7\text{F}^-$                                            | −0.45                              |                         |  |
| <b>Technetium</b>                                                                                      |                                    |                         |  |
| $\text{TcO}_4^- + 4\text{H}^+ + 3\text{e}^- = \text{TcO}_2 + 2\text{H}_2\text{O}$                      | 0.738                              |                         |  |
| $\text{TcO}_4^- + 2\text{H}^+ + \text{e}^- = \text{TcO}_3 + \text{H}_2\text{O}$                        | 0.700                              |                         |  |
| $\text{TcO}_4^- + \text{e}^- = \text{TcO}_4^{2-}$                                                      | 0.569                              |                         |  |
| $\text{TcO}_4^- + 8\text{H}^+ + 7\text{e}^- = \text{Tc} + 4\text{H}_2\text{O}$                         | 0.472                              |                         |  |
| $\text{TcO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- = \text{TcO}_2 + 2\text{H}_2\text{O}$                   | 1.39                               |                         |  |
| $\text{TcO}_2 + 4\text{H}^+ + 4\text{e}^- = \text{Tc} + 2\text{H}_2\text{O}$                           | 0.272                              |                         |  |
| $\text{Tc} + \text{e}^- = \text{Tc}^-$                                                                 | ca. −0.5                           |                         |  |
| <b>Tellurium</b>                                                                                       |                                    |                         |  |
| $\text{H}_2\text{TeO}_4 + 6\text{H}^+ + 2\text{e}^- = \text{Te}^{4+} + 4\text{H}_2\text{O}$            | 0.929                              |                         |  |
| $\text{H}_2\text{TeO}_4 + 2\text{H}^+ + 2\text{e}^- = \text{TeO}_2(\text{c}) + 2\text{H}_2\text{O}$    | 1.02                               |                         |  |
| $\text{TeO}_4^{2-} + 2\text{H}^+ + 2\text{e}^- = \text{TeO}_3^{2-} + \text{H}_2\text{O}$               | 0.897                              |                         |  |
| $\text{TeOOH}^+ + 3\text{H}^+ + 4\text{e}^- = \text{Te} + 2\text{H}_2\text{O}$                         | 0.559                              |                         |  |
| $\text{H}_2\text{TeO}_3 + 4\text{H}^+ + 4\text{e}^- = \text{Te} + 3\text{H}_2\text{O}$                 | 0.589                              |                         |  |
| $\text{TeO}_3^{2-} + 6\text{H}^+ + 4\text{e}^- = \text{Te} + 3\text{H}_2\text{O}$                      | 0.827                              |                         |  |
| $\text{TeO}_3^{2-} + 3\text{H}_2\text{O} + 4\text{e}^- = \text{Te} + 6\text{OH}^-$                     | −0.415                             |                         |  |
| $\text{TeO}_2(\text{c}) + 4\text{H}^+ + 4\text{e}^- = \text{Te} + 2\text{H}_2\text{O}$                 | 0.521                              |                         |  |
| $\text{Te} + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{Te}(\text{aq})$                               | −0.740                             |                         |  |
| $\text{Te} + \text{H}^+ + 2\text{e}^- = \text{HTe}^-$                                                  | −0.817                             |                         |  |
| $\text{Te}^{2-} + 2\text{H}^+ + 2\text{e}^- = 2\text{HTe}^-$                                           | −0.794                             |                         |  |
| <b>Terbium</b>                                                                                         |                                    |                         |  |
| $\text{Tb}^{3+} + 3\text{e}^- = \text{Tb}$                                                             | −2.31                              |                         |  |
| <b>Thallium</b>                                                                                        |                                    |                         |  |
| $\text{Tl}^{3+} + 2\text{e}^- = \text{Tl}^+$                                                           | 1.25                               |                         |  |
|                                                                                                        | 0.77                               |                         |  |
| $\text{Tl}^{3+} + 3\text{e}^- = \text{Tl}$                                                             | 0.72                               |                         |  |
| $\text{Tl}^+ + \text{e}^- = \text{Tl}$                                                                 | −0.336                             |                         |  |
| $\text{TlCl} + \text{e}^- = \text{Tl} + \text{Cl}^-$                                                   | −0.557                             |                         |  |
| $\text{TlBr} + \text{e}^- = \text{Tl} + \text{Br}^-$                                                   | −0.658                             |                         |  |
| $\text{TlI} + \text{e}^- = \text{Tl} + \text{I}^-$                                                     | −0.752                             |                         |  |
| <b>Thorium</b>                                                                                         |                                    |                         |  |
| $\text{Th}^{4+} + 4\text{e}^- = \text{Th}$                                                             | −1.83                              |                         |  |



**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                          | Standard<br>or formal<br>potential | Solution<br>composition |
|----------------------------------------------------------------------------------------|------------------------------------|-------------------------|
| <b>Thullium</b>                                                                        |                                    |                         |
| $\text{Tm}^{3+} + 3e^- = \text{Tm}$                                                    | -2.32                              |                         |
| <b>Tin</b>                                                                             |                                    |                         |
| $\text{Sn}^{4+} + 2e^- = \text{Sn}^{2+}$                                               | 0.154                              |                         |
| $\text{SnCl}_6^{2-} + 2e^- = \text{SnCl}_4^{2-} + 2\text{Cl}^-$                        | 0.14                               |                         |
| $\text{SnO}_3^{2-} + 6\text{H}^+ + 2e^- = \text{Sn}^{2+} + 3\text{H}_2\text{O}$        | 0.849                              |                         |
| $\text{SnF}_6^{2-} + 4e^- = \text{Sn} + 6\text{F}^-$                                   | -0.200                             |                         |
| $\text{Sn}^{2+} + 2e^- = \text{Sn}$                                                    | -0.1375                            |                         |
| $\text{SnCl}_4^{2-} + 2e^- = \text{Sn} + 4\text{Cl}^-$                                 | -0.19                              | 1 HCl                   |
| $\text{HSnO}_2 + \text{H}_2\text{O} + 2e^- = \text{Sn} + 3\text{OH}^-$                 | -0.91                              |                         |
| $\text{Sn} + 4\text{H}^+ + 4e^- = \text{SnH}_4$                                        | -1.07                              |                         |
| <b>Titanium</b>                                                                        |                                    |                         |
| $\text{TiO}^{2+} + 2\text{H}^+ + e^- = \text{Ti}^{3+} + \text{H}_2\text{O}$            | -0.10                              |                         |
| $\text{TiO}^{2+} + 2\text{H}^+ + 4e^- = \text{Ti} + \text{H}_2\text{O}$                | -0.86                              |                         |
| $\text{Ti}^{3+} + e^- = \text{Ti}^{2+}$                                                | -0.37                              |                         |
| $\text{Ti}^{3+} + 3e^- = \text{Ti}$                                                    | -1.21                              |                         |
| $\text{Ti}^{2+} + 2e^- = \text{Ti}$                                                    | -1.63                              |                         |
| <b>Tungsten</b>                                                                        |                                    |                         |
| $2\text{WO}_3 + 2\text{H}^+ + 2e^- = \text{W}_2\text{O}_5 + \text{H}_2\text{O}$        | -0.029                             |                         |
| $\text{WO}_3 + 6\text{H}^+ + 6e^- = \text{W} + 3\text{H}_2\text{O}$                    | -0.090                             |                         |
| $\text{WO}_4^{2-} + 4\text{H}_2\text{O} + 6e^- = \text{W} + 8\text{OH}^-$              | -1.074                             |                         |
| $\text{WO}_4^{2-} + 2\text{H}_2\text{O} + 2e^- = \text{WO}_2 + 4\text{OH}^-$           | -1.259                             |                         |
| $\text{W}_2\text{O}_5 + 2\text{H}^+ + 2e^- = 2\text{WO}_2 + \text{H}_2\text{O}$        | -0.031                             |                         |
| $\text{W}(\text{CN})_8^{3-} + e^- = \text{W}(\text{CN})_8^{4-}$                        | 0.457                              |                         |
| $\text{WO}_2 + 4\text{H}^+ + 4e^- = \text{W} + 2\text{H}_2\text{O}$                    | -0.119                             |                         |
| $\text{WO}_2 + 2\text{H}_2\text{O} + 4e^- = \text{W} + 4\text{OH}^-$                   | -0.982                             |                         |
| <b>Uranium</b>                                                                         |                                    |                         |
| $\text{UO}_2^{2+} + e^- = \text{UO}_2^+$                                               | 0.16                               |                         |
| $\text{UO}_2^{2+} + 4\text{H}^+ + 2e^- = \text{U}^{4+} + 2\text{H}_2\text{O}$          | 0.27                               |                         |
| $\text{UO}_2^+ + 4\text{H}^+ + e^- = \text{U}^{4+} + 2\text{H}_2\text{O}$              | 0.38                               |                         |
| $\text{U}^{4+} + e^- = \text{U}^{3+}$                                                  | -0.52                              |                         |
| $\text{U}^{4+} + 4e^- = \text{U}$                                                      | -1.38                              |                         |
| $\text{U}^{3+} + 3e^- = \text{U}$                                                      | -1.66                              |                         |
| <b>Vanadium</b>                                                                        |                                    |                         |
| $\text{VO}_2^+ + 2\text{H}^+ + e^- = \text{VO}^{2+} + \text{H}_2\text{O}$              | 1.000                              |                         |
| $\text{VO}_2^+ + 4\text{H}^+ + 2e^- = \text{V}^{3+} + 2\text{H}_2\text{O}$             | 0.668                              |                         |
| $\text{VO}_2^+ + 4\text{H}^+ + 3e^- = \text{V}^{2+} + 2\text{H}_2\text{O}$             | 0.361                              |                         |
| $\text{VO}_2^+ + 4\text{H}^+ + 5e^- = \text{V} + 4\text{H}_2\text{O}$                  | -0.236                             |                         |
| $\text{VO}^{2+} + 2\text{H}^+ + e^- = \text{V}^{3+} + \text{H}_2\text{O}$              | 0.337                              |                         |
| $\text{V}^{3+} + e^- = \text{V}^{2+}$                                                  | -0.255                             |                         |
| $\text{V}^{2+} + 2e^- = \text{V}$                                                      | -1.13                              |                         |
| <b>Xenon</b>                                                                           |                                    |                         |
| $\text{H}_4\text{XeO}_6 + 2\text{H}^+ + 2e^- = \text{XeO}_3 + 3\text{H}_2\text{O}$     | 2.42                               |                         |
| $\text{HXeO}_6^{3-} + 2\text{H}_2\text{O} + e^- = \text{HXeO}_4 + 4\text{OH}^-$        | 0.9                                |                         |
| $\text{XeO}_3 + 6\text{H}^+ + 2\text{F}^- + 4e^- = \text{XeF}_2 + 3\text{H}_2\text{O}$ | 1.6                                |                         |
| $\text{XeO}_3 + 6\text{H}^+ + 6e^- = \text{Xe}(\text{g}) + 3\text{H}_2\text{O}$        | 2.10                               |                         |
| $\text{XeF}_2 + e^- = \text{XeF} + \text{F}^-$                                         | 0.9                                |                         |
| $\text{XeF}_2 + 2\text{H}^+ + 2e^- = \text{Xe}(\text{g}) + 2\text{HF}$                 | 2.64                               |                         |
| $\text{XeF} + e^- = \text{Xe}(\text{g}) + \text{F}^-$                                  | 3.4                                |                         |

**TABLE 8.27** Potentials of the Elements and Their Compounds at 25°C (*Continued*)

| Half-reaction                                                                    | Standard or formal potential | Solution composition |
|----------------------------------------------------------------------------------|------------------------------|----------------------|
| <b>Ytterbium</b>                                                                 |                              |                      |
| $\text{Yb}^{3+} + e^- = \text{Yb}^{2+}$                                          | -1.05                        |                      |
| $\text{Yb}^{2+} + 2e^- = \text{Yb}$                                              | -2.8                         |                      |
| $\text{Yb}^{3+} + 3e^- = \text{Yb}$                                              | -2.22                        |                      |
| <b>Yttrium</b>                                                                   |                              |                      |
| $\text{Y}^{3+} + 3e^- = \text{Y}$                                                | -2.37                        |                      |
| <b>Zinc</b>                                                                      |                              |                      |
| $\text{Zn}^{2+} + 2e^- = \text{Zn}$                                              | -0.7626                      |                      |
| $\text{Zn}(\text{NH}_3)_4^{2+} + 2e^- = \text{Zn} + 4\text{NH}_3$                | -1.04                        |                      |
| $\text{Zn}(\text{CN})_4^{2-} + 2e^- = \text{Zn} + 4\text{CN}^-$                  | -1.34                        |                      |
| $\text{Zn}(\text{tartrate})_4^{6-} + 2e^- = \text{Zn} + 4(\text{tartrate})^{2-}$ | -1.15                        |                      |
| $\text{Zn}(\text{OH})_4^{2-} + 2e^- = \text{Zn} + 4\text{OH}^-$                  | -1.285                       |                      |
| <b>Zirconium</b>                                                                 |                              |                      |
| $\text{Zr}^{4+} + 4e^- = \text{Zr}$                                              | -1.55                        |                      |
| $\text{ZrO}_2 + 4\text{H}^+ + 4e^- = \text{Zr} + 2\text{H}_2\text{O}$            | -1.45                        |                      |

**TABLE 8.28** Potentials of Selected Half-Reactions at 25°C

A summary of oxidation-reduction half-reactions arranged in order of decreasing oxidation strength and useful for selecting reagent systems.

| Half-reaction                                                                                         | $E^\circ$ , volts |
|-------------------------------------------------------------------------------------------------------|-------------------|
| $\text{F}_2(\text{g}) + 2\text{H}^+ + 2e^- = 2\text{HF}$                                              | 3.053             |
| $\text{O}_3 + \text{H}_2\text{O} + 2e^- = \text{O}_2 + 2\text{OH}^-$                                  | 1.246             |
| $\text{O}_3 + 2\text{H}^+ + 2e^- = \text{O}_2 + \text{H}_2\text{O}$                                   | 2.075             |
| $\text{Ag}^{2+} + e^- = \text{Ag}^+$                                                                  | 1.980             |
| $\text{S}_2\text{O}_8^{2-} + 2e^- = 2\text{SO}_4^{2-}$                                                | 1.96              |
| $\text{HN}_3 + 3\text{H}^+ + 2e^- = \text{NH}_4^+ + \text{N}_2$                                       | 1.96              |
| $\text{H}_2\text{O}_2 + 2\text{H}^+ + 2e^- = 2\text{H}_2\text{O}$                                     | 1.763             |
| $\text{Ce}^{4+} + e^- = \text{Ce}^{3+}$                                                               | 1.72              |
| $\text{MnO}_4^- + 4\text{H}^+ + 3e^- = \text{MnO}_2(\text{c}) + 2\text{H}_2\text{O}$                  | 1.70              |
| $2\text{HClO} + 2\text{H}^+ + 2e^- = \text{Cl}_2 + \text{H}_2\text{O}$                                | 1.630             |
| $2\text{HBrO} + 2\text{H}^+ + 2e^- = \text{Br}_2 + \text{H}_2\text{O}$                                | 1.604             |
| $\text{H}_5\text{IO}_6 + \text{H}^+ + 2e^- = \text{IO}_3^- + 3\text{H}_2\text{O}$                     | 1.603             |
| $\text{NiO}_2 + 4\text{H}^+ + 2e^- = \text{Ni}^{2+} + 2\text{H}_2\text{O}$                            | 1.593             |
| $\text{Bi}_2\text{O}_4(\text{bismuthate}) + 4\text{H}^+ + 2e^- = 2\text{BiO}^+ + 2\text{H}_2\text{O}$ | 1.59              |
| $\text{MnO}_4^- + 8\text{H}^+ + 5e^- = \text{Mn}^{2+} + 4\text{H}_2\text{O}$                          | 1.51              |
| $2\text{BrO}_3^- + 12\text{H}^+ + 10e^- = \text{Br}_2 + 6\text{H}_2\text{O}$                          | 1.478             |
| $\text{PbO}_2 + 4\text{H}^+ + 2e^- = \text{Pb}^{2+} + 2\text{H}_2\text{O}$                            | 1.468             |
| $\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6e^- = 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$            | 1.36              |
| $\text{Cl}_2 + 2e^- = 2\text{Cl}^-$                                                                   | 1.3583            |
| $2\text{HNO}_2 + 4\text{H}^+ + 4e^- = \text{N}_2\text{O} + 3\text{H}_2\text{O}$                       | 1.297             |
| $\text{N}_2\text{H}_5^+ + 3\text{H}^+ + 2e^- = 2\text{NH}_4^+$                                        | 1.275             |
| $\text{MnO}_2 + 4\text{H}^+ + 2e^- = \text{Mn}^{2+} + 2\text{H}_2\text{O}$                            | 1.23              |
| $\text{O}_2 + 4\text{H}^+ + 4e^- = 2\text{H}_2\text{O}$                                               | 1.229             |
| $\text{ClO}_4^- + 2\text{H}^+ + 2e^- = \text{ClO}_3^- + \text{H}_2\text{O}$                           | 1.201             |

**TABLE 8.28** Potentials of Selected Half-Reactions at 25°C (*Continued*)

| Half-reaction                                                                                          | $E^\circ$ , volts |
|--------------------------------------------------------------------------------------------------------|-------------------|
| $2\text{IO}_3^- + 12\text{H}^+ + 10\text{e}^- = \text{I}_2 + 3\text{H}_2\text{O}$                      | 1.195             |
| $\text{N}_2\text{O}_4 + 2\text{H}^+ + 2\text{e}^- = 2\text{HNO}_3$                                     | 1.07              |
| $2\text{ICl}_2^- + 2\text{e}^- = 4\text{Cl}^- + \text{I}_2$                                            | 1.07              |
| $\text{Br}_2(\text{lq}) + 2\text{e}^- = 2\text{Br}^-$                                                  | 1.065             |
| $\text{N}_2\text{O}_4 + 4\text{H}^+ + 4\text{e}^- = 2\text{NO} + 2\text{H}_2\text{O}$                  | 1.039             |
| $\text{HNO}_2 + \text{H}^+ + \text{e}^- = \text{NO} + \text{H}_2\text{O}$                              | 0.996             |
| $\text{NO}_3^- + 4\text{H}^+ + 3\text{e}^- = \text{NO} + 2\text{H}_2\text{O}$                          | 0.957             |
| $\text{NO}_3^- + 3\text{H}^+ + 2\text{e}^- = \text{HNO}_2 + \text{H}_2\text{O}$                        | 0.94              |
| $2\text{Hg}^{2+} + 2\text{e}^- = \text{Hg}_2^{2+}$                                                     | 0.911             |
| $\text{Cu}^{2+} + \text{I}^- + \text{e}^- = \text{CuI}$                                                | 0.861             |
| $\text{OsO}_4(\text{c}) + 8\text{H}^+ + 8\text{e}^- = \text{Os} + 4\text{H}_2\text{O}$                 | 0.84              |
| $\text{Ag}^+ + \text{e}^- = \text{Ag}$                                                                 | 0.7991            |
| $\text{Hg}_2^{2+} + 2\text{e}^- = 2\text{Hg}$                                                          | 0.7960            |
| $\text{Fe}^{3+} + \text{e}^- = \text{Fe}^{2+}$                                                         | 0.771             |
| $\text{H}_2\text{SeO}_3 + 4\text{H}^+ + 4\text{e}^- = \text{Se} + 3\text{H}_2\text{O}$                 | 0.739             |
| $\text{HN}_3 + 11\text{H}^+ + 8\text{e}^- = 2\text{NH}_4^+$                                            | 0.695             |
| $\text{O}_2 + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{O}_2$                                        | 0.695             |
| $\text{Ag}_2\text{SO}_4 + 2\text{e}^- = 2\text{Ag} + \text{SO}_4^{2-}$                                 | 0.654             |
| $\text{Cu}^{2+} + \text{Br}^- + \text{e}^- = \text{CuBr}(\text{c})$                                    | 0.654             |
| $\text{Au}(\text{SCN})_4^- + 3\text{e}^- = \text{Au} + 4\text{SCN}^-$                                  | 0.636             |
| $2\text{HgCl}_2 + 2\text{e}^- = \text{Hg}_2\text{Cl}_2(\text{c}) + 2\text{Cl}^-$                       | 0.63              |
| $\text{Sb}_2\text{O}_5 + 6\text{H}^+ + 4\text{e}^- = 2\text{SbO}^+ + 3\text{H}_2\text{O}$              | 0.605             |
| $\text{H}_3\text{AsO}_4 + 2\text{H}^+ + 2\text{e}^- = \text{HAsO}_2 + 2\text{H}_2\text{O}$             | 0.560             |
| $\text{TeOOH}^+ + 3\text{H}^+ + 4\text{e}^- = \text{Te} + 2\text{H}_2\text{O}$                         | 0.559             |
| $\text{Cu}^{2+} + \text{Cl}^- + \text{e}^- = \text{CuCl}(\text{c})$                                    | 0.559             |
| $\text{I}_3^- + 2\text{e}^- = 3\text{I}^-$                                                             | 0.536             |
| $\text{I}_2 + 2\text{e}^- = 2\text{I}^-$                                                               | 0.536             |
| $\text{Cu}^+ + \text{e}^- = \text{Cu}$                                                                 | 0.53              |
| $4\text{H}_2\text{SO}_3 + 4\text{H}^+ + 6\text{e}^- = \text{S}_4\text{O}_6^{2-} + 6\text{H}_2\text{O}$ | 0.507             |
| $\text{Ag}_2\text{CrO}_4 + 2\text{e}^- = 2\text{Ag} + \text{CrO}_4^{2-}$                               | 0.449             |
| $2\text{H}_2\text{SO}_3 + 2\text{H}^+ + 4\text{e}^- = \text{S}_2\text{O}_3^{2-} + 3\text{H}_2\text{O}$ | 0.400             |
| $\text{UO}_2^{2+} + 4\text{H}^+ + \text{e}^- = \text{U}^{4+} + 2\text{H}_2\text{O}$                    | 0.38              |
| $\text{Fe}(\text{CN})_6^{3-} + \text{e}^- = \text{Fe}(\text{CN})_6^{4-}$                               | 0.361             |
| $\text{Cu}^{2+} + 2\text{e}^- = \text{Cu}$                                                             | 0.340             |
| $\text{VO}^{2+} + 2\text{H}^+ + \text{e}^- = \text{V}^{3+} + \text{H}_2\text{O}$                       | 0.337             |
| $\text{BiO}^+ + 2\text{H}^+ + 3\text{e}^- = \text{Bi} + \text{H}_2\text{O}$                            | 0.32              |
| $\text{UO}_2^{2+} + 4\text{H}^+ + 2\text{e}^- = \text{U}^{4+} + 2\text{H}_2\text{O}$                   | 0.27              |
| $\text{Hg}_2\text{Cl}_2(\text{c}) + 2\text{e}^- = 2\text{Hg} + 2\text{Cl}^-$                           | 0.2676            |
| $\text{AgCl} + \text{e}^- = \text{Ag} + \text{Cl}^-$                                                   | 0.2223            |
| $\text{SbO}^+ + 2\text{H}^+ + 3\text{e}^- = \text{Sb} + \text{H}_2\text{O}$                            | 0.212             |
| $\text{CuCl}_3^{2-} + \text{e}^- = \text{Cu} + 3\text{Cl}^-$                                           | 0.178             |
| $\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- = \text{H}_2\text{SO}_3 + \text{H}_2\text{O}$            | 0.158             |
| $\text{Sn}^{4+} + 2\text{e}^- = \text{Sn}^{2+}$                                                        | 0.15              |
| $\text{S} + 2\text{H}^+ + 2\text{e}^- = \text{H}_2\text{S}$                                            | 0.144             |
| $\text{Hg}_2\text{Br}_2(\text{c}) + 2\text{e}^- = 2\text{Hg} + 2\text{Br}^-$                           | 0.1392            |
| $\text{CuCl} + \text{e}^- = \text{Cu} + \text{Cl}^-$                                                   | 0.121             |
| $\text{TiO}^{2+} + 2\text{H}^+ + \text{e}^- = \text{Ti}^{3+} + \text{H}_2\text{O}$                     | 0.100             |
| $\text{S}_4\text{O}_6^{2-} + 2\text{e}^- = 2\text{S}_2\text{O}_3^{2-}$                                 | 0.08              |
| $\text{AgBr} + \text{e}^- = \text{Ag} + \text{Br}^-$                                                   | 0.0711            |
| $\text{HCOOH} + 2\text{H}^+ + 2\text{e}^- = \text{HCHO} + \text{H}_2\text{O}$                          | 0.056             |
| $\text{CuBr} + \text{e}^- = \text{Cu} + \text{Br}^-$                                                   | 0.033             |
| $2\text{H}^+ + 2\text{e}^- = \text{H}_2$                                                               | 0.0000            |
| $\text{Hg}_2\text{I}_2 + 2\text{e}^- = 2\text{Hg} + 2\text{I}^-$                                       | -0.0405           |

**TABLE 8.28** Potentials of Selected Half-Reactions at 25°C (*Continued*)

| Half-reaction                                                                               | $E^\circ$ , volts |
|---------------------------------------------------------------------------------------------|-------------------|
| $\text{Pb}^{2+} + 2e^- = \text{Pb}$                                                         | -0.125            |
| $\text{Sn}^{2+} + 2e^- = \text{Sn}$                                                         | -0.136            |
| $\text{AgI} + e^- = \text{Ag} + \text{I}^-$                                                 | -0.1522           |
| $\text{N}_2 + 5\text{H}^+ + 4e^- = \text{N}_2\text{H}_5^+$                                  | -0.225            |
| $\text{V}^{3+} + e^- = \text{V}^{2+}$                                                       | -0.255            |
| $\text{Ni}^{2+} + 2e^- = \text{Ni}$                                                         | -0.257            |
| $\text{Co}^{2+} + 2e^- = \text{Co}$                                                         | -0.277            |
| $\text{Ag}(\text{CN})_2^- + e^- = \text{Ag} + 2\text{CN}^-$                                 | -0.31             |
| $\text{PbSO}_4 + 2e^- = \text{Pb} + \text{SO}_4^{2-}$                                       | -0.3505           |
| $\text{Cd}^{2+} + 2e^- = \text{Cd}$                                                         | -0.4025           |
| $\text{Cr}^{3+} + e^- = \text{Cr}^{2+}$                                                     | -0.424            |
| $\text{Fe}^{2+} + 2e^- = \text{Fe}$                                                         | -0.44             |
| $\text{H}_3\text{PO}_3 + 2\text{H}^+ + 2e^- = \text{H}_2\text{PO}_2^- + \text{H}_2\text{O}$ | -0.499            |
| $2\text{CO}_2 + 2\text{H}^+ + 2e^- = \text{H}_2\text{C}_2\text{O}_4$                        | -0.49             |
| $\text{U}^{4+} + e^- = \text{U}^{3+}$                                                       | -0.52             |
| $\text{Zn}^{2+} + 2e^- = \text{Zn}$                                                         | -0.7626           |
| $\text{Mn}^{2+} + 2e^- = \text{Mn}$                                                         | -1.18             |
| $\text{Al}^{3+} + 3e^- = \text{Al}$                                                         | -1.67             |
| $\text{Mg}^{2+} + 2e^- = \text{Mg}$                                                         | -2.356            |
| $\text{Na}^+ + e^- = \text{Na}$                                                             | -2.714            |
| $\text{K}^+ + e^- = \text{K}$                                                               | -2.925            |
| $\text{Li}^+ + e^- = \text{Li}$                                                             | -3.045            |
| $3\text{N}_2 + 2\text{H}^+ + 2e^- = 2\text{HN}_3$                                           | -3.10             |

**TABLE 8.29** Overpotentials for Common Electrode Reactions at 25°C

The overpotential is defined as the difference between the actual potential of an electrode at a given current density and the reversible electrode potential for the reaction.

| Electrode                                                              | Current Density, A/cm <sup>2</sup> |       |        |       |       |       |
|------------------------------------------------------------------------|------------------------------------|-------|--------|-------|-------|-------|
|                                                                        | 0.001                              | 0.01  | 0.1    | 0.5   | 1.0   | 5.0   |
|                                                                        | Overpotential, volts               |       |        |       |       |       |
| <b>Liberation of H<sub>2</sub> from 1M H<sub>2</sub>SO<sub>4</sub></b> |                                    |       |        |       |       |       |
| Ag                                                                     | 0.097                              | 0.13  | 0.3    |       | 0.48  | 0.69  |
| Al                                                                     | 0.3                                | 0.83  | 1.00   |       | 1.29  |       |
| Au                                                                     | 0.017                              |       | 0.1    |       | 0.24  | 0.33  |
| Bi                                                                     | 0.39                               | 0.4   |        |       | 0.78  | 0.98  |
| Cd                                                                     |                                    | 1.13  | 1.22   |       | 1.25  |       |
| Co                                                                     |                                    | 0.2   |        |       |       |       |
| Cr                                                                     |                                    | 0.4   |        |       |       |       |
| Cu                                                                     |                                    |       | 0.35   |       | 0.48  | 0.55  |
| Fe                                                                     |                                    | 0.56  | 0.82   |       | 1.29  |       |
| Graphite                                                               | 0.002                              |       | 0.32   |       | 0.60  | 0.73  |
| Hg                                                                     | 0.8                                | 0.93  | 1.03   |       | 1.07  |       |
| Ir                                                                     | 0.0026                             | 0.2   |        |       |       |       |
| Ni                                                                     | 0.14                               | 0.3   |        |       | 0.56  | 0.71  |
| Pb                                                                     | 0.40                               | 0.4   |        |       | 0.52  | 1.06  |
| Pd                                                                     | 0                                  | 0.04  |        |       |       |       |
| Pt (smooth)                                                            | 0.0000                             | 0.16  | 0.29   |       | 0.68  |       |
| Pt (platinized)                                                        | 0.0000                             | 0.030 | 0.041  |       | 0.048 | 0.051 |
| Sb                                                                     |                                    | 0.4   |        |       |       |       |
| Sn                                                                     |                                    | 0.5   | 1.2    |       |       |       |
| Ta                                                                     |                                    | 0.39  | 0.4    |       |       |       |
| Zn                                                                     | 0.48                               | 0.75  | 1.06   |       | 1.23  |       |
| <b>Liberation of O<sub>2</sub> from 1M KOH</b>                         |                                    |       |        |       |       |       |
| Ag                                                                     | 0.58                               | 0.73  | 0.98   |       | 1.13  |       |
| Au                                                                     | 0.67                               | 0.96  | 1.24   |       | 1.63  |       |
| Cu                                                                     | 0.42                               | 0.58  | 0.66   |       | 0.79  |       |
| Graphite                                                               | 0.53                               | 0.90  | 1.09   |       | 1.24  |       |
| Ni                                                                     | 0.35                               | 0.52  | 0.73   |       | 0.85  |       |
| Pt (smooth)                                                            | 0.72                               | 0.85  | 1.28   |       | 1.49  |       |
| Pt (platinized)                                                        | 0.40                               | 0.52  | 0.64   |       | 0.77  |       |
| <b>Liberation of Cl<sub>2</sub> from saturated NaCl solution</b>       |                                    |       |        |       |       |       |
| Graphite                                                               |                                    |       | 0.25   | 0.42  | 0.53  |       |
| Platinized Pt                                                          | 0.006                              |       | 0.026  | 0.05  |       |       |
| Smooth Pt                                                              | 0.008                              | 0.03  | 0.054  | 0.161 | 0.236 |       |
| <b>Liberation of Br<sub>2</sub> from saturated NaBr solution</b>       |                                    |       |        |       |       |       |
| Graphite                                                               |                                    | 0.002 | 0.027  | 0.16  | 0.33  |       |
| Platinized Pt                                                          |                                    | 0.002 | 0.012  | 0.069 | 0.21  |       |
| Smooth Pt                                                              |                                    | 0.002 | 0.006* | 0.26  | 0.38† |       |
| <b>Liberation of I<sub>2</sub> from saturated NaI solution</b>         |                                    |       |        |       |       |       |
| Graphite                                                               | 0.002                              | 0.014 | 0.097  |       |       |       |
| Platinized Pt                                                          |                                    | 0.006 | 0.032  |       | 0.196 |       |
| Smooth Pt                                                              |                                    | 0.003 | 0.03   | 0.12  | 0.22  |       |

\* At 0.23 A/cm<sup>2</sup>.      † At 0.72 A/cm<sup>2</sup>.

The overpotential required for the evolution of O<sub>2</sub> from dilute solutions of HClO<sub>4</sub>, HNO<sub>3</sub>, H<sub>3</sub>PO<sub>4</sub> or H<sub>2</sub>SO<sub>4</sub> onto smooth platinum electrodes is approximately 0.5 V.

**TABLE 8.30** Half-Wave Potentials of Inorganic Materials*All values are in volts vs. the saturated calomel electrode.*

| Element                                                  | $E_{1/2}$ , volts                                         | Solvent system                                                                                                                                                                                                                |
|----------------------------------------------------------|-----------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Aluminum</b><br>3+                                    | -0.5                                                      | 0.2M acetate, pH 4.5–4.7, plus 0.07% azo dye Pontochrome Violet SW; reduction wave of complexed dye is 0.2 V more negative than that of the free dye.                                                                         |
| <b>Antimony</b><br>3+ to 0                               | -0.15<br>-0.31(1)<br>-0.8<br>-1.0; -1.2<br>-1.26<br>-1.32 | 1M HCl<br>1M HNO <sub>3</sub> (or 0.5M H <sub>2</sub> SO <sub>4</sub> )<br>0.5M tartrate, pH 4.5<br>0.5M tartrate, pH 9 (waves not distinct)<br>1M NaOH; also anodic wave (3+ to 5+) at -0.45<br>0.5M tartrate plus 0.1M NaOH |
| 5+                                                       | 0.0; -0.257                                               | 6M HCl. First wave (5+ to 3+) starts at the oxidation potential of Hg; second wave is 3+ to 0.                                                                                                                                |
| 5+ to 0                                                  | -0.35                                                     | 1M HCl plus 4M KBr                                                                                                                                                                                                            |
| <b>Arsenic</b><br>3+ to 5+<br>3+                         | -0.26<br>-0.8; -1.0<br>-0.7; -1.0                         | 0.5M KOH (anodic wave); only suitable wave<br>0.1M HCl; ill-defined waves<br>0.5M H <sub>2</sub> SO <sub>4</sub> (or 1M HNO <sub>3</sub> )                                                                                    |
| <b>Barium</b><br>2+ to 0                                 | -1.94                                                     | 0.1M (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> NI                                                                                                                                                                         |
| <b>Bismuth</b><br>3+ to 0                                | -0.025(15)<br>-0.09<br>-0.29<br>-0.7<br>-1.0              | 1M HNO <sub>3</sub> (or 0.5M H <sub>2</sub> SO <sub>4</sub> )<br>1M HCl<br>0.5M tartrate, pH 4.5<br>0.5M tartrate (pH 9), wave not well-developed<br>0.5M tartrate plus 0.1M NaOH, poor wave                                  |
| <b>Bromine</b><br>5+ to 1-<br>0 to 1-<br>Br <sup>-</sup> | -1.75<br>0.13<br>0.0<br>0.1                               | 0.1M alkali chlorides (or 0.1M NaOH)<br>0.05M H <sub>2</sub> SO <sub>4</sub><br>Wave (anodic) starts at zero; Hg <sub>2</sub> Br <sub>2</sub> forms<br>Oxidation of Hg to form mercury(I) bromide                             |
| <b>Cadmium</b><br>2+ to 0                                | -0.60<br>-0.64<br>-0.81                                   | 0.1M KCl, or 0.5M H <sub>2</sub> SO <sub>4</sub> , or 1M HNO <sub>3</sub><br>0.5M tartrate at pH 4.5 or 9<br>1M NH <sub>4</sub> Cl plus 1M NH <sub>3</sub>                                                                    |
| <b>Calcium</b><br>2+ to 0                                | -2.22<br>-2.13                                            | 0.1M (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> NCl<br>0.1M (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> NCl in 80% ethanol                                                                                               |
| <b>Cerium</b><br>3+ to 0                                 | -1.97                                                     | 0.02M alkali sulfate                                                                                                                                                                                                          |
| <b>Cesium</b><br>1+ to 0                                 | -2.05                                                     | 0.1M (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> NOH in 50% ethanol                                                                                                                                                         |
| <b>Chlorine</b><br>Cl <sup>-</sup>                       | 0.25                                                      | Oxidation of Hg to form Hg <sub>2</sub> Cl <sub>2</sub>                                                                                                                                                                       |
| <b>Chromium</b><br>6+ to 3+<br>3+ to 0<br>3+ to 2+       | -0.85<br>-0.35; -1.70<br>-0.95                            | CrO <sub>4</sub> <sup>2-</sup> to CrO <sub>2</sub> <sup>-</sup> in 0.1 to 1M NaOH<br>1M NH <sub>4</sub> Cl—NH <sub>3</sub> buffer (pH 8–9); 3+ to 2+ to 0<br>0.1M pyridine–0.1M pyridinium chloride                           |

**TABLE 8.30** Half-Wave Potentials of Inorganic Materials (*Continued*)

| Element                      | $E_{1/2}$ , volts | Solvent system                                                                                        |
|------------------------------|-------------------|-------------------------------------------------------------------------------------------------------|
| 2+ to 0                      | -1.54             | 1M KCl                                                                                                |
| 2+ to 3+                     | -0.40             | 1M KCl (anodic wave)                                                                                  |
| <b>Cobalt</b>                |                   |                                                                                                       |
| 3+ to 0                      | -0.5; -1.3        | 1M NH <sub>4</sub> Cl plus 1M NH <sub>3</sub> ; 3+ to 2+ to 0                                         |
| 2+ to 0                      | -1.07             | 0.1M pyridine plus pyridinium chloride                                                                |
|                              | -1.03             | Neutral 1M potassium thiocyanate                                                                      |
|                              | -1.4              | Co(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> in noncomplexing systems                              |
| 3+ to 2+                     | 0.0               | 1M sodium oxalate in acetate buffer (pH 5); diffusion current measured between 0 and -0.1 V           |
| <b>Copper</b>                |                   |                                                                                                       |
| 2+ to 0                      | 0.04              | 0.1M KNO <sub>3</sub> , 0.1M NH <sub>4</sub> ClO <sub>4</sub> , or 1M Na <sub>2</sub> SO <sub>4</sub> |
|                              | -0.085            | 0.1M Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub> plus 0.2M Na acetate, pH 4.5                       |
|                              | -0.09             | 0.5M Na tartrate, pH 4.5                                                                              |
|                              | -0.20             | 0.1M potassium oxalate, pH 5.7 to 10                                                                  |
|                              | -0.22             | 0.5M potassium citrate, pH 7.5                                                                        |
|                              | -0.4              | 0.5M Na tartrate plus 0.1M NaOH (pH 12)                                                               |
|                              | -0.568            | 0.1M KNO <sub>3</sub> plus 1M ethylenediamine                                                         |
| 2+                           | 0.04; -0.22       | 1M KCl; consecutive waves: 2+ to 1+ to 0                                                              |
|                              | -0.02; -0.39      | 0.1M KSCN; consecutive waves: 2+ to 1+ to 0                                                           |
|                              | 0.05; -0.25       | 0.1M pyridine plus 0.1M pyridinium chloride; consecutive waves: 2+ to 1+ to 0                         |
|                              | -0.24; -0.50      | 1M NH <sub>4</sub> Cl plus 1M NH <sub>3</sub> ; consecutive waves                                     |
| <b>Gallium</b>               |                   |                                                                                                       |
| 3+ to 0                      | -1.1              | Not more than 0.001M HCl or wave masked by hydrogen wave which immediately follows                    |
| <b>Germanium</b>             |                   |                                                                                                       |
| 2+ to 0                      | -0.45             | 6M HCl; prior reduction with HPH <sub>2</sub> O <sub>2</sub> to 2+                                    |
| <b>Gold</b>                  |                   |                                                                                                       |
| 3+ to 1+                     | 0                 | 1M KCN; wave starts at 0 V                                                                            |
| 1+ to 0                      | -1.4              | Au(CN) <sub>2</sub> <sup>-</sup> wave best for analytical purposes                                    |
| <b>Indium</b>                |                   |                                                                                                       |
| 3+ to 0                      | -0.60             | 1M KCl<br>In Na acetate, pH 3.9 to 4.2                                                                |
| <b>Iodine</b>                |                   |                                                                                                       |
| IO <sub>4</sub> <sup>-</sup> | 0.36              | First wave at pH 0 (shifts to -0.08 at pH 12); second wave corresponds to iodate reduction            |
| IO <sub>3</sub> <sup>-</sup> | -0.075            | 0.2M KNO <sub>3</sub> (shifts -0.13 V/pH unit increase)                                               |
|                              | -0.305            | 0.1M hydrogen phthalate, pH 3.2                                                                       |
|                              | -0.500            | 0.1M acetate plus 0.1M KCl, pH 4.9                                                                    |
|                              | -0.650            | 0.1M citrate, pH 5.95                                                                                 |
|                              | -1.050            | 0.2M phosphate, pH 7.10                                                                               |
|                              | -1.20             | 0.05M borax + 0.1M KCl, pH 9.2; or NaOH plus 0.1M KCl, pH 13.0                                        |
| 0 to 1-                      | 0.0               | Wave starts from zero in acid media; Hg <sub>2</sub> I <sub>2</sub> formed                            |
| 1-                           | -0.1              | Oxidation of Hg to form Hg <sub>2</sub> I <sub>2</sub>                                                |
| <b>Iron</b>                  |                   |                                                                                                       |
| 3+                           | -0.44; -1.52      | 1M (NH <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub> ; two waves; 3+ to 2+ to 0                         |
|                              | -0.17; -1.50      | 0.5M Na tartrate, pH 5.8; two waves; 3+ to 2+ to 0                                                    |
|                              | -0.9; -1.5        | 0.1 to 5M KOH plus 8% mannitol; 3+ to 2+ to 0                                                         |

**TABLE 8.30** Half-Wave Potentials of Inorganic Materials (*Continued*)

| Element                | $E_{1/2}$ , volts                              | Solvent system                                                                                                                                                                                                                               |
|------------------------|------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 3+ to 2+               | -0.13<br>-0.27<br>-0.28<br>-1.46(2)<br>-1.36   | 0.1M EDTA plus 2M Na acetate, pH 6-7<br>0.2M Na oxalate, pH 7.9 or less<br>0.5M Na citrate, pH 6.5<br>1M $\text{NH}_4\text{ClO}_4$<br>0.1M $\text{KHF}_2$ , pH 4 or less                                                                     |
| 2+ to 3+               | -0.28<br>-0.27<br>-0.17<br>-1.36               | 0.5M Na citrate, pH 6.5<br>0.2M Na oxalate, pH 7.9 or less<br>0.5M Na tartrate, pH 5.8<br>0.1M $\text{KHF}_2$ , pH 4 or less                                                                                                                 |
| <b>Lead</b>            |                                                |                                                                                                                                                                                                                                              |
| 2+ to 0                | -0.405<br>-0.435<br>-0.49(1)<br>-0.72<br>-0.75 | 1M $\text{HNO}_3$<br>1M KCl (or HCl)<br>0.5M Na tartrate, pH 4.5 or 9<br>1M KCN<br>1M KOH or 0.5M Na tartrate plus 0.1M NaOH                                                                                                                 |
| <b>Lithium</b>         |                                                |                                                                                                                                                                                                                                              |
| 1+ to 0                | -2.31                                          | 0.1M $(\text{C}_2\text{H}_5)_4\text{NOH}$ in 50% ethanol                                                                                                                                                                                     |
| <b>Magnesium</b>       |                                                |                                                                                                                                                                                                                                              |
| 2+ to 0                | -2.2                                           | 0.1M $(\text{C}_2\text{H}_5)_4\text{NCl}$ (poorly defined wave)                                                                                                                                                                              |
| <b>Manganese</b>       |                                                |                                                                                                                                                                                                                                              |
| 2+ to 0                | -1.65<br>-1.55<br>-1.33                        | 1M $\text{NH}_4\text{Cl}$ plus 1M $\text{NH}_3$<br>1M KCNS<br>1.5M KCN                                                                                                                                                                       |
| <b>Molybdenum</b>      |                                                |                                                                                                                                                                                                                                              |
| 6+                     | -0.26; -0.63                                   | 0.3M HCl, two waves: 6+ to 5+ to 3+                                                                                                                                                                                                          |
| <b>Nickel</b>          |                                                |                                                                                                                                                                                                                                              |
| 2+ to 0                | -0.70<br>-0.78<br>-1.09<br>-1.1<br>-1.36       | 1M KSCN<br>1M KCl plus 0.5M pyridine<br>1M $\text{NH}_4\text{Cl}$ plus 1M $\text{NH}_3$<br>$\text{Ni}(\text{H}_2\text{O})_6^{2+}$ in $\text{NH}_4\text{ClO}_4$ or $\text{KNO}_3$<br>$\text{Ni}(\text{CN})_4^{2-}$ in 1M KCN (alkaline media) |
| <b>Niobium</b>         |                                                |                                                                                                                                                                                                                                              |
| 5+ to 3+               | -0.80(4)                                       | 1M $\text{HNO}_3$                                                                                                                                                                                                                            |
| <b>Nitrogen</b>        |                                                |                                                                                                                                                                                                                                              |
| Nitrate                | -1.45                                          | 0.017M $\text{LaCl}_3$ (reduced to hydroxylamine)                                                                                                                                                                                            |
| $\text{HNO}_2$         | -0.77                                          | 0.1M HCl                                                                                                                                                                                                                                     |
| $\text{C}_2\text{N}_2$ | -1.2; -1.55                                    | 0.1M Na acetate, two waves                                                                                                                                                                                                                   |
| Oxamic acid            | -1.55                                          | 0.1M Na acetate                                                                                                                                                                                                                              |
| Cyanide                | -0.45                                          | 0.1M NaOH; anodic wave starts at -0.45                                                                                                                                                                                                       |
| Thiocyanate            | 0.18                                           | Anodic wave; neutral or weakly alkaline medium                                                                                                                                                                                               |
| <b>Osmium</b>          |                                                |                                                                                                                                                                                                                                              |
| $\text{OsO}_4$         | 0.0; -0.41;<br>-1.16                           | Sat'd $\text{Ca}(\text{OH})_2$ . Three waves: first starts at 0; second wave is $\text{OsO}_4^{2-}$ to Os(V); and third wave is Os(V) to Os(III)                                                                                             |
| <b>Oxygen</b>          |                                                |                                                                                                                                                                                                                                              |
| $\text{O}_2$           | -0.05; -0.9                                    | Buffer solutions of pH 1 to 10. Two waves: $\text{O}_2$ to $\text{H}_2\text{O}_2$ , and $\text{H}_2\text{O}_2$ to $\text{H}_2\text{O}$ . Second wave extends from -0.5 to -1.3                                                               |
| $\text{H}_2\text{O}_2$ | -0.9                                           | Very extended wave (see above); sharper in presence of Aerosol OT                                                                                                                                                                            |



**TABLE 8.30** Half-Wave Potentials of Inorganic Materials (*Continued*)

| Element                                                                                                                  | $E_{1/2}$ , volts                                | Solvent system                                                                                                                                                                                                                                         |
|--------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Palladium</b><br>2+ to 0                                                                                              | -0.31<br>-0.64<br>-0.72                          | 1M pyridine plus 1M KCl<br>0.1M ethylenediamine plus 1M KCl<br>1M $\text{NH}_4\text{Cl}$ plus 1M $\text{NH}_3$                                                                                                                                         |
| <b>Potassium</b><br>1+ to 0                                                                                              | -2.10                                            | 0.1M $(\text{C}_2\text{H}_5)_4\text{NOH}$ in 50% ethanol                                                                                                                                                                                               |
| <b>Rhenium</b><br>7+ to 4+<br>4+ to 3+                                                                                   | -0.44<br>-0.51                                   | 2M HCl or (better) 4M $\text{HClO}_4$<br>$\text{ReCl}_6^{2-}$ ion in 1M HCl                                                                                                                                                                            |
| <b>Rhodium</b><br>3+ to 2+                                                                                               | -0.41                                            | 1M pyridine plus 1M KCl                                                                                                                                                                                                                                |
| <b>Rubidium</b><br>1+ to 0                                                                                               | -1.99                                            | 0.1M $(\text{C}_2\text{H}_5)_4\text{NOH}$ in 50% ethanol                                                                                                                                                                                               |
| <b>Scandium</b><br>3+ to 0                                                                                               | -1.80                                            | 0.1M LiCl, KCl, or $\text{BaCl}_2$                                                                                                                                                                                                                     |
| <b>Selenium</b><br>4+ to 2-<br>2-                                                                                        | -1.44<br>-1.54<br>-0.49<br>-0.94                 | 1M $\text{NH}_4\text{Cl}$ plus $\text{NH}_3$ , pH 8.0<br>Same system adjusted to pH 9.5<br>Anodic wave at pH 0 due to HgSe<br>Anodic wave at pH 12 (0.01M NaOH)                                                                                        |
| <b>Silver</b><br>1+ to 0<br>1+ to 0                                                                                      | -0.3                                             | Wave starts at oxidation potential of Hg<br>0.0014M $\text{KAg}(\text{CN})_2$ without excess cyanide                                                                                                                                                   |
| <b>Sodium</b><br>1+ to 0                                                                                                 | -2.07                                            | 0.1M $(\text{C}_2\text{H}_5)_4\text{NOH}$ in 50% ethanol                                                                                                                                                                                               |
| <b>Strontium</b><br>2+ to 0                                                                                              | -2.11                                            | 0.1M $(\text{C}_2\text{H}_5)_4\text{NI}$ , water or 80% ethanol                                                                                                                                                                                        |
| <b>Sulfur</b><br>$\text{SO}_2$<br>$\text{S}_2\text{O}_4^{2-}$<br>$\text{S}_2\text{O}_3^{2-}$<br>0 to 2-<br>$\text{HS}^-$ | -0.38<br>-0.43<br>-0.15<br>-0.50<br>-0.76        | 1M $\text{HNO}_3$ (or other strong acid); 4+ to 2+<br>0.5M $(\text{NH}_4)_2\text{HPO}_4$ plus 1M $\text{NH}_3$ (anodic wave)<br>1M strong acid; anodic mercury wave<br>90% methanol, 9.5% pyridine, 0.5% HCl (pH 6)<br>0.1M NaOH (anodic mercury wave) |
| <b>Tellurium</b><br>4+ to 0<br>4+ to 2-<br>2- to 0                                                                       | -0.4<br>-0.63<br>-1.22<br>-0.72<br>-0.08         | Citrate buffer, pH 1.6 (second of two waves)<br>Ammoniacal buffer, pH 9.4<br>0.1M NaOH<br>1M HCl (true anodic reversible wave)<br>1M NaOH (same as above; intermediate values at pH 1 to 13)                                                           |
| <b>Thallium</b><br>3+ to 0                                                                                               | -0.48                                            | 1M KCl, $\text{KNO}_3$ , $\text{K}_2\text{SO}_4$ , KOH, or $\text{NH}_3$                                                                                                                                                                               |
| <b>Tin</b><br>4+ to 2+<br>2+ to 0<br>2+ to 4+                                                                            | -0.25; -0.52<br>-0.59<br>-1.22<br>-0.28<br>-0.73 | 4M $\text{NH}_4\text{Cl}$ + 1M HCl; two waves: 4+ to 2+ to 0<br>0.5M tartrate, pH 4.3<br>1M NaOH (stannite ion to tin)<br>0.5M Na tartrate, pH 4.3 (anodic wave)<br>1M NaOH (stannite ion to stannate ion)                                             |

**TABLE 8.30** Half-Wave Potentials of Inorganic Materials (*Continued*)

| Element                           | $E_{1/2}$ , volts                                   | Solvent system                                                                                                                    |
|-----------------------------------|-----------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| <b>Titanium</b><br>4+ to 3+       | -0.173<br>-1.22                                     | 0.1M K <sub>2</sub> C <sub>2</sub> O <sub>4</sub> plus 1M H <sub>2</sub> SO <sub>4</sub><br>0.4M tartrate, pH 6.5                 |
| <b>Tungsten</b><br>6+             | 0.0; -0.64                                          | 6M HCl; two waves: first wave starts at zero and is W(VI) to W(V), the second wave is W(V) to W(III)                              |
| <b>Uranium</b><br>6+              | -0.180; -0.92                                       | UO <sub>2</sub> <sup>2+</sup> to UO <sub>2</sub> <sup>+</sup> , then U <sup>3+</sup> in 0.02M HCL                                 |
| <b>Vanadium</b><br>5+ to 4+ to 2+ | -0.97; -1.26                                        | 1M NH <sub>4</sub> Cl plus 1M NH <sub>3</sub> and 0.08M Na <sub>2</sub> SO <sub>3</sub>                                           |
| 4+ to 2+                          | -0.98                                               | 0.05M H <sub>2</sub> SO <sub>4</sub>                                                                                              |
| 3+ to 2+                          | -0.55                                               | 0.5M H <sub>2</sub> SO <sub>4</sub>                                                                                               |
| 4+ to 5+                          | -0.32                                               | 1M NH <sub>4</sub> Cl, 1M NH <sub>3</sub> , and 0.08M Na <sub>2</sub> SO <sub>3</sub>                                             |
| 4+ to 5+                          | 0.76                                                | 0.05M H <sub>2</sub> SO <sub>4</sub> ; anodic wave starting from zero                                                             |
| 2+ to 3+                          | -0.55                                               | 0.5M H <sub>2</sub> SO <sub>4</sub> ; anodic wave                                                                                 |
| <b>Zinc</b><br>2+ to 0            | -0.995<br>-1.01<br>-1.15<br>-1.23<br>-1.33<br>-1.53 | 0.1M KCl<br>0.1M KSCN<br>0.5M tartrate, pH 9<br>0.5M tartrate, pH 4.5<br>1M NH <sub>4</sub> Cl plus 1M NH <sub>3</sub><br>1M NaOH |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C

The solvent systems in this table are listed below:

A, acetonitrile and a perchlorate salt such as  $\text{LiClO}_4$  or a tetraalkyl ammonium salt

B, acetic acid and an alkali acetate, often plus a tetraalkyl ammonium iodide

C, 0.05 to 0.175M tetraalkyl ammonium halide and 75% 1,4-dioxane

D, buffer plus 50% ethanol (EtOH)

**Abbreviations Used in the Table**

|               |                |
|---------------|----------------|
| Bu, butyl     | Me, methyl     |
| Et, ethyl     | MeOH, methanol |
| EtOH, ethanol | PrOH, propanol |
| M, molar      |                |

| Compound                                    | Solvent system                        | $E_{1/2}$           |
|---------------------------------------------|---------------------------------------|---------------------|
| Unsaturated aliphatic hydrocarbons          |                                       |                     |
| Acrylonitrile                               | C but 30% EtOH                        | −1.94               |
| Allene                                      | C                                     | −2.29               |
| 1,3-Butadiene                               | A                                     | −2.03               |
|                                             | C                                     | −2.59               |
| 1,3-Butadiyne                               | C                                     | −1.89               |
| 1-Buten-2-yne                               | C                                     | −2.40               |
| 1,4-Cyclohexadiene                          | A                                     | −1.6                |
| Cyclohexene                                 | A                                     | −1.89               |
| 1,3,5,7-Cyclooctatetraene                   | B                                     | −1.42               |
|                                             | C                                     | −1.51               |
| Diethyl fumarate                            | B, pH 4.0                             | −0.84               |
| Diethyl maleate                             | B, pH 4.0                             | −0.95               |
| 2,3-Dimethyl-1,3-butadiene                  | A                                     | −1.83               |
| Dimethylfulvene                             | C                                     | −1.89               |
| Diphenylacetylene                           | C                                     | −2.20               |
| 1,1-Diphenylethylene                        | B                                     | −1.52               |
|                                             | C                                     | −2.19               |
| Ethyl methacrylate                          | 0.1 N $\text{LiCl}$ + 25% EtOH        | −1.9                |
| 2-Methyl-1,3-butadiene                      | A                                     | −1.84               |
| 2-Methyl-1-butene                           | A                                     | −1.97               |
| 1-Piperidino-4-cyano-4-phenyl-1,3-butadiene | $\text{LiClO}_4$ in dimethylformamide | −0.16               |
| <i>trans</i> -Stilbene                      | B                                     | −1.51               |
| Tetrakis(dimethylamino)ethylene             | A                                     | −0.75               |
| Aromatic hydrocarbons                       |                                       |                     |
| Acenaphthene                                | A                                     | −0.95               |
|                                             | B                                     | −1.36               |
|                                             | C                                     | −2.58               |
| Anthracene                                  | A                                     | −0.84               |
|                                             | B                                     | −1.20               |
|                                             | C                                     | −1.94               |
| Azulene                                     | A                                     | −0.71               |
|                                             | C                                     | −1.66, −2.26, −2.56 |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                          | Solvent system | $E_{1/2}$      |
|-----------------------------------|----------------|----------------|
| Aromatic hydrocarbons (continued) |                |                |
| 1,2-Benzanthracene                | C              | − 2.03, − 2.54 |
| 2,3-Benzanthracene                | A              | − 0.54, − 1.20 |
| Benzene                           | A              | − 2.08         |
| 1,2-Benzo[ <i>a</i> ]pyrene       | A              | − 0.76         |
| Biphenyl                          | A              | − 1.48         |
|                                   | B              | − 1.91         |
|                                   | C              | − 2.70         |
| Chrysene                          | A              | − 1.22         |
| 1,2,5,6-Dibenzanthracene          | A              | − 1.00, − 1.26 |
| 1,2-Dihydronaphthalene            | C              | − 2.57         |
| 9,10-Dimethylantracene            | A              | − 0.65         |
| 2,3-Dimethylnaphthalene           | A              | − 1.08, − 1.34 |
| 9,10-Diphenylantracene            | A              | − 0.92         |
| Fluorene                          | A              | − 1.25         |
|                                   | B              | − 1.65         |
|                                   | C              | − 2.65         |
| Hexamethylbenzene                 | A              | − 1.16         |
|                                   | B              | − 1.52         |
| Indan                             | A              | − 1.59, − 2.02 |
| Indene                            | A              | − 1.23         |
|                                   | C              | − 2.81         |
| 1-Methylnaphthalene               | A              | − 1.24         |
|                                   | B              | − 1.53         |
|                                   | C              | − 2.46         |
| 2-Methylnaphthalene               | A              | − 1.22         |
|                                   | B              | − 1.55         |
|                                   | C              | − 2.46         |
| Naphthalene                       | A              | − 1.34         |
|                                   | B              | − 1.72         |
| Pentamethylbenzene                | A              | − 1.28         |
|                                   | B              | − 1.62         |
| Phenanthrene                      | A              | − 1.23         |
|                                   | B              | − 1.68         |
|                                   | C              | − 2.46, − 2.71 |
| Phenylacetylene                   | C              | − 2.37         |
| Pyrene                            | A              | − 1.06, − 1.24 |
| <i>trans</i> -Stilbene            | B              | − 1.51         |
|                                   | C              | − 2.26         |
| Styrene                           | C              | − 2.35         |
| 1,2,3,5-Tetramethylbenzene        | A              | − 1.50, − 1.99 |
| 1,2,4,5-Tetramethylbenzene        | A              | − 1.29         |
| Tetraphenylethylene               | C              | − 2.05         |
| 1,4,5,8-Tetraphenylnaphthalene    | A              | − 1.39         |
| Toluene                           | A              | − 1.98         |
| 1,2,3-Trimethylbenzene            | A              | − 1.58         |
| 1,2,4-Trimethylbenzene            | A              | − 1.41         |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                          | Solvent system                  | $E_{1/2}$              |
|-----------------------------------|---------------------------------|------------------------|
| Aromatic hydrocarbons (continued) |                                 |                        |
| 1,3,5-Trimethylbenzene            | A                               | − 1.50                 |
|                                   | B                               | − 1.90                 |
| Triphenylene                      | A                               | − 1.46, − 1.55         |
| Triphenylmethane                  | C                               | − 1.01, − 1.68, − 1.96 |
| <i>o</i> -Xylene                  | A                               | − 1.58, − 2.04         |
| <i>m</i> -Xylene                  | A                               | − 1.58                 |
| <i>p</i> -Xylene                  | A                               | − 1.56                 |
| Aldehydes                         |                                 |                        |
| Acetaldehyde                      | B, pH 6.8–13                    | − 1.89                 |
| Benzaldehyde                      | McIlvaine buffer, pH 2.2        | − 0.96, − 1.32         |
| Bromoacetaldehyde                 | pH 8.5                          | − 0.40                 |
|                                   | pH 9.8                          | − 1.58, − 1.82         |
| Chloroacetaldehyde                | Ammonia buffer, pH 8.4          | − 1.06, − 1.66         |
| Cinnamaldehyde                    | Buffer + EtOH, pH 6.0           | − 0.9, − 1.5, − 1.7    |
| Crotonaldehyde                    | B, pH 1.3–2.0                   | − 0.92                 |
|                                   | Ammonia buffer, pH 8.0          | − 1.30                 |
| Dichloroacetaldehyde              | Ammonia buffer, pH 8.4          | − 1.03, − 1.67         |
| 3,7-Dimethyl-2,6-octadienal       | 0.1 M Et <sub>4</sub> NI        | − 1.56, − 2.22         |
| Formaldehyde                      | 0.05 M KOH+0.1 M KCl, pH 12.7   | − 1.59                 |
| 2-Furaldehyde                     | pH 1–8                          | − 0.86–0.07 pH         |
|                                   | pH 10                           | − 1.43                 |
| Glucose                           | Phosphate buffer, pH 7          | − 1.55                 |
| Glyceraldehyde                    | Britton-Robinson buffer, pH 5.0 | − 1.47                 |
|                                   | Britton-Robinson buffer, pH 8.0 | − 1.55                 |
| Glycolaldehyde                    | 0.1 M KOH, pH 13                | − 1.70                 |
| Glyoxal                           | B, pH 3.4                       | − 1.41                 |
| 4-Hydroxybenzaldehyde             | Britton-Robinson buffer, pH 1.8 | − 1.16                 |
|                                   | Britton-Robinson buffer, pH 6.8 | − 1.45                 |
| 4-Hydroxy-2-methoxybenzaldehyde   | McIlvaine buffer, pH 2.2        | − 1.05                 |
|                                   | McIlvaine buffer, pH 5.0        | − 1.16, − 1.36         |
|                                   | McIlvaine buffer, pH 8.0        | − 1.47                 |
| <i>o</i> -Methoxybenzaldehyde     | Britton-Robinson buffer, pH 1.8 | − 1.02                 |
|                                   | Britton-Robinson buffer, pH 6.8 | − 1.49                 |
| <i>p</i> -Methoxybenzaldehyde     | Britton-Robinson buffer, pH 1.8 | − 1.17                 |
|                                   | Britton-Robinson buffer, pH 6.8 | − 1.48                 |
| Methyl glyoxal                    | A, pH 4.5                       | − 0.83                 |
| <i>m</i> -Nitrobenzaldehyde       | Buffer +10% EtOH, pH 2.0        | − 0.28, − 1.20         |
| Phthalaldehyde                    | Buffer, pH 3.1                  | − 0.64, − 1.07         |
|                                   | Buffer, pH 7.3                  | − 0.89, − 1.29         |
| 2-Propenal (acrolein)             | pH 4.5                          | − 1.36                 |
|                                   | pH 9.0                          | − 1.1                  |
| Propionaldehyde                   | 0.1 M LiOH, pH 13               | − 1.93                 |
| Pyrrole-2-carbaldehyde            | 0.1 M HCl+50% EtOH              | − 1.25                 |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                                     | Solvent system                                                                                                                 | $E_{1/2}$                                  |
|----------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------|
| Aldehydes ( <i>continued</i> )               |                                                                                                                                |                                            |
| Salicylaldehyde                              | McIlvaine buffer, pH 2.2<br>McIlvaine buffer, pH 5.0<br>McIlvaine buffer, pH 8.0                                               | - 0.99, - 1.23<br>- 1.20, - 1.30<br>- 1.32 |
| Trichloroacetaldehyde                        | Ammonia buffer, pH 8.4<br>0.1 M KCl + 50% EtOH                                                                                 | - 1.35, - 1.66<br>- 1.55                   |
| Ketones                                      |                                                                                                                                |                                            |
| Acetone                                      | B, pH 9.3<br>C                                                                                                                 | - 1.52<br>- 2.46                           |
| Acetophenone                                 | D + McIlvaine buffer, pH 4.9<br>D + McIlvaine buffer, pH 7.2<br>D + McIlvaine buffer, pH 1.3                                   | - 1.33<br>- 1.58<br>- 1.08                 |
| 7 <i>H</i> -Benz[ <i>de</i> ]anthracen-7-one | 0.1 N H <sub>2</sub> SO <sub>4</sub> + 75% MeOH                                                                                | - 0.96                                     |
| Benzil                                       | D + McIlvaine buffer, pH 1.3<br>D + McIlvaine buffer, pH 4.9                                                                   | - 0.27<br>- 0.50                           |
| Benzoin                                      | D + McIlvaine buffer, pH 1.3<br>D + McIlvaine buffer, pH 8.6                                                                   | - 0.90<br>- 1.49                           |
| Benzophenone                                 | D + McIlvaine buffer, pH 1.3<br>D + McIlvaine buffer, pH 8.6                                                                   | - 0.94<br>- 1.36                           |
| Benzoylacetone                               | Buffer, pH 2.6<br>Buffer, pH 5.3 and pH 7.6<br>Buffer, pH 9.7                                                                  | - 1.60<br>- 1.68<br>- 1.72                 |
| Bromoacetone                                 | 0.1 M LiCl                                                                                                                     | - 0.29                                     |
| 2,3-Butanedione                              | 0.1 M HCl                                                                                                                      | - 0.84                                     |
| 3-Buten-2-one                                | 0.1 M KCl                                                                                                                      | - 1.42                                     |
| Butyrophenone                                | 0.1 M NH <sub>4</sub> Cl + 50% EtOH                                                                                            | - 1.55                                     |
| D-Carvone                                    | 0.1 M Et <sub>4</sub> Ni + 80% EtOH                                                                                            | - 1.71                                     |
| Chloroacetone                                | 0.1 M LiCl                                                                                                                     | - 1.18                                     |
| Coumarin                                     | McIlvaine buffer, pH 2.0<br>McIlvaine buffer, pH 5.0                                                                           | - 0.95<br>- 1.11, - 1.44                   |
| Cyclohexanone                                | C                                                                                                                              | - 2.45                                     |
| <i>cis</i> -Dibenzoylethylene                | D, pH 1                                                                                                                        | - 0.30                                     |
| <i>trans</i> -Dibenzoylethylene              | D, pH 11<br>D, pH 1                                                                                                            | - 0.62, - 1.65<br>- 0.12                   |
| Dibenzoylmethane                             | D, pH 11<br>D, pH 1.3                                                                                                          | - 0.57, - 1.52<br>- 0.59                   |
| 9,10-Dihydro-9-oxoanthracene                 | D, pH 11.3                                                                                                                     | - 1.30, - 1.62                             |
| 1,5-Diphenyl-1,5-pentanedione                | D, pH 2.0                                                                                                                      | - 0.93                                     |
| 1,5-Diphenylthiocarbazone                    | A<br>D, pH 7.0                                                                                                                 | - 2.10<br>- 0.6                            |
| Flavanone                                    | Acetate buffer + Me <sub>4</sub> NOH + 50%<br>2-ProOH, pH 6.1<br>Acetate buffer + Me <sub>4</sub> NOH + 50%<br>2-ProOH, pH 9.6 | - 1.30<br>- 1.51                           |
| Fluorescein                                  | Acetate buffer, pH 2.0<br>Phthalate buffer, pH 5.0<br>Borate buffer, pH 10.1                                                   | - 0.50<br>- 0.65<br>- 1.18, - 1.44         |
| Fructose                                     | 0.02 M LiCl                                                                                                                    | - 1.76                                     |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                                | Solvent system                          | $E_{1/2}$              |
|-----------------------------------------|-----------------------------------------|------------------------|
| Ketones (continued)                     |                                         |                        |
| Girard derivatives of aliphatic ketones | pH 8.2                                  | − 1.52                 |
| <i>o</i> -Hydroxyacetophenone           | D, pH 5                                 | − 1.36                 |
| <i>p</i> -Hydroxyacetophenone           | D, pH 5                                 | − 1.46                 |
| 1,2,3-Indantrione (ninhydrin)           | Britton-Robinson buffer, pH 2.5         | − 0.67, − 0.83         |
|                                         | Britton-Robinson buffer, pH 4.5         | − 0.73, − 1.01         |
|                                         | Britton-Robinson buffer, pH 6.8         | − 0.10, − 0.90, − 1.20 |
|                                         | Britton-Robinson buffer, pH 9.2         | − 1.35                 |
| $\alpha$ -Ionone                        | C                                       | − 1.59, − 2.08         |
| Isatin                                  | Phosphate buffer+citrate buffer, pH 2.9 | − 0.3, − 0.5           |
|                                         | Phosphate buffer+citrate buffer, pH 4.3 | − 0.3, − 0.5, − 0.8    |
|                                         | Phosphate buffer+citrate buffer, pH 5.4 | − 0.8                  |
| 4-Methyl-3,5-heptadien-2-one            | A                                       | − 0.64                 |
| 4-Methyl-2,6-heptanedione               | A                                       | − 1.28                 |
| 4-Methyl-3-penten-2-one                 | D+McIlvaine buffer, pH 1.3              | − 1.01                 |
|                                         | D+McIlvaine buffer, pH 11.3             | − 1.60                 |
| 4-Phenyl-3-buten-2-one                  | D, pH 1.3                               | − 0.72                 |
|                                         | D, pH 8.6                               | − 1.27                 |
| Phthalide                               | 0.1 M Bu <sub>4</sub> NI + 50% dioxane  | − 0.20                 |
| Phthalimide                             | pH 4.2                                  | − 1.1, − 1.5           |
|                                         | pH 9.7                                  | − 1.2, − 1.4           |
| Pulegone                                | C                                       | − 1.74                 |
| Quinalizarin                            | Phosphate buffer+1% EtOH, pH 8.0        | − 0.56                 |
| Testosterone                            | D+Britton-Robinson buffer, pH 2.6       | − 1.20                 |
|                                         | D+Britton-Robinson buffer, pH 5.8       | − 1.40                 |
|                                         | D+Britton-Robinson buffer, pH 8.8       | − 1.53, − 1.79         |
| Quinones                                |                                         |                        |
| Anthraquinone                           | Acetate buffer+40% dioxane, pH 5.6      | − 0.51                 |
|                                         | Phosphate buffer+40% dioxane, pH 7.9    | − 0.71                 |
| <i>o</i> -Benzoquinone                  | Britton-Robinson buffer, pH 7.0         | + 0.20                 |
|                                         | Britton-Robinson buffer, pH 9.0         | + 0.08                 |
| 2,3-Dimethylnaphthoquinone              | D, pH 5.4                               | − 0.22                 |
| 1,2-Naphthoquinone                      | Phosphate buffer, pH 5.0                | − 0.03                 |
|                                         | Phosphate buffer, pH 7.0                | − 0.13                 |
| 1,4-Naphthoquinone                      | Britton-Robinson buffer, pH 7.0         | − 0.07                 |
|                                         | Britton-Robinson buffer, pH 9.0         | − 0.19                 |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                     | Solvent system                                | $E_{1/2}$           |
|------------------------------|-----------------------------------------------|---------------------|
| Acids                        |                                               |                     |
| Acetic acid                  | A                                             | -2.3                |
| Acrylic acid                 | pH 5.6                                        | -0.85               |
| Adenosine-5'-phosphoric acid | HClO <sub>4</sub> +KClO <sub>4</sub> , pH 2.2 | -1.13               |
| 4-Aminobenzenesulfonic acid  | 0.05 M Me <sub>4</sub> NI                     | -1.58               |
| 3-Aminobenzoic acid          | pH 5.6                                        | -0.67               |
| Anthranilic acid             | pH 5.6                                        | -0.67               |
| Ascorbic acid                | Britton-Robinson buffer, pH 3.4               | +0.17               |
|                              | Britton-Robinson buffer, pH 7.0               | -0.06               |
| Barbituric acid              | Borate buffer, pH 9.3                         | -0.04               |
| Benzoic acid                 | A                                             | -2.1                |
| Benzoylformic acid           | Britton-Robinson buffer, pH 2.2               | -0.48               |
|                              | Britton-Robinson buffer, pH 5.5               | -0.85, -1.26        |
|                              | Britton-Robinson buffer, pH 7.2               | -0.98, -1.25        |
|                              | Britton-Robinson buffer, pH 9.2               | -1.25               |
| Bromoacetic acid             | pH 1.1                                        | -0.54               |
| 2-Bromopropionic acid        | pH 2.0                                        | -0.39               |
| Crotonic acid                | C                                             | -1.94               |
| Dibromoacetic acid           | pH 1.1                                        | -0.03, -0.59        |
| Dichloroacetic acid          | pH 8.2                                        | -1.57               |
| 5,5-Diethylbarbituric acid   | Borate buffer, pH 9.3                         | 0.00                |
| Flavanol                     | D, pH 5.6                                     | -1.25               |
|                              | D, pH 7.7                                     | -1.40               |
| Folic acid                   | Britton-Robinson buffer, pH 4.6               | -0.73               |
| Formic acid                  | 0.1 M KCl                                     | -1.66               |
| Fumaric acid                 | HCl+KCl, pH 2.6                               | -0.83               |
|                              | Acetate buffer, pH 4.0                        | -0.93               |
|                              | Acetate buffer, pH 5.9                        | -1.20               |
| 2,4-Hexadienedioic acid      | Acetate buffer, pH 4.5                        | -0.97               |
| Iodoacetic acid              | pH 1                                          | -0.16               |
| Maleic acid                  | Britton-Robinson buffer, pH 2.0               | -0.70               |
|                              | Britton-Robinson buffer, pH 4.0               | -0.97               |
|                              | Britton-Robinson buffer, pH 6.0               | -1.11, -1.30        |
|                              | Britton-Robinson buffer, pH 10.0              | -1.51               |
| Mercaptoacetic acid          | B, pH 6.8                                     | -0.38               |
| Methacrylic acid             | D+0.1 M LiCl                                  | -1.69               |
| Nitrobenzoic acids           | Buffer+10% EtOH, pH 2.0                       | -0.2, -0.7          |
| Oxalic acid                  | B, pH 5.4-6.1                                 | -1.80               |
| 2-Oxo-1,5-pentanedioic acid  | HCl+KCl, pH 1.8                               | -0.59               |
|                              | Ammonia buffer, pH 8.2                        | -1.30               |
| 2-Oxopropionic acid          | Britton-Robinson buffer, pH 5.6               | -1.17               |
|                              | Britton-Robinson buffer, pH 6.8               | -1.22, -1.53        |
|                              | Britton-Robinson buffer, pH 9.7               | -1.51               |
| Phenolphthalein              | Phthalate buffer, pH 2.5                      | -0.67               |
|                              | Phthalate buffer, pH 4.7                      | -0.80               |
|                              | D, pH 9.6                                     | -0.98, -1.35        |
| Picric acid                  | pH 4.2                                        | -0.34               |
|                              | pH 11.7                                       | -0.36, -0.56, -0.96 |



**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(*Continued*)

| Compound                                       | Solvent system                       | $E_{1/2}$    |
|------------------------------------------------|--------------------------------------|--------------|
| <i>Acids (continued)</i>                       |                                      |              |
| 1,2,3-Propenetricarboxylic acid                | pH 7.0                               | -2.1         |
| Trichloroacetic acid                           | Ammonia buffer, pH 8.2               | -0.84, -1.57 |
|                                                | Phosphate buffer, pH 10.4            | -0.9, -1.6   |
| 3,4,5-Trihydroxybenzoic acid                   | Phosphate buffer, pH 2.9             | +0.50        |
|                                                | Phosphate buffer, pH 8.8             | +0.1         |
| <i>p</i> -Aminophenol                          | Britton-Robinson buffer, pH 6.3      | +0.14        |
|                                                | Britton-Robinson buffer, pH 8.6      | -0.04        |
|                                                | Britton-Robinson buffer, pH 12.0     | -0.16        |
| <i>o</i> -Chlorophenol                         | pH 5.6                               | -0.63        |
| <i>m</i> -Chlorophenol                         | pH 5.6                               | -0.73        |
| <i>p</i> -Chlorophenol                         | pH 5.6                               | -0.65        |
| <i>o</i> -Cresol                               | pH 5.6                               | -0.56        |
| <i>m</i> -Cresol                               | pH 5.6                               | -0.61        |
| <i>p</i> -Cresol                               | pH 5.6                               | -0.54        |
| 1,2-Dihydroxybenzene                           | pH 5.6                               | -0.35        |
| 1,3-Dihydroxybenzene                           | pH 5.6                               | -0.61        |
| 1,4-Dihydroxybenzene                           | pH 5.6                               | -0.23        |
| <i>o</i> -Methoxyphenol                        | pH 5.6                               | -0.46        |
| <i>m</i> -Methoxyphenol                        | pH 5.6                               | -0.62        |
| <i>p</i> -Methoxyphenol                        | pH 5.6                               | -0.41        |
| 1-Naphthol                                     | A                                    | -0.74        |
| 2-Naphthol                                     | A                                    | -0.82        |
| 1,2,3-Trihydroxybenzene                        | Britton-Robinson buffer, pH 3.1      | +0.35        |
|                                                | Britton-Robinson buffer, pH 6.5      | +0.10        |
|                                                | Britton-Robinson buffer, pH 9.5      | -0.10        |
| <i>Halogen compounds</i>                       |                                      |              |
| Bromobenzene                                   | A                                    | -1.98        |
|                                                | C                                    | -2.32        |
| 1-Bromobutane                                  | C                                    | -2.27        |
| Bromoethane                                    | C                                    | -2.08        |
| Bromomethane                                   | C                                    | -1.63        |
| 1-Bromonaphthalene (also 2-bromonaphthalene)   | A                                    | -1.55, -1.60 |
| 3-Bromo-1-propene                              | C                                    | -1.29        |
| <i>p</i> -Bromotoluene                         | A                                    | -1.72        |
| Carbon tetrachloride                           | C                                    | -0.78, -1.71 |
| Chlorobenzene                                  | A                                    | -2.07        |
| Chloroform                                     | C                                    | -1.63        |
| Chloromethane                                  | C                                    | -2.23        |
| 3-Chloro-1-propene                             | C                                    | -1.91        |
| $\alpha$ -Chlorotoluene                        | C                                    | -1.81        |
| <i>p</i> -Chlorotoluene                        | A                                    | -1.76        |
| <i>N</i> -Chloro- <i>p</i> -toluenesulfonamide | 0.5 M K <sub>2</sub> SO <sub>4</sub> | -0.13        |
| 9,10-Dibromoanthracene                         | A                                    | -1.15, -1.47 |
| <i>p</i> -Dibromobenzene                       | C                                    | -2.10        |
| 1,2-Dibromobutane                              | D+1% Na <sub>2</sub> SO <sub>3</sub> | -1.45        |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                                 | Solvent system                           | $E_{1/2}$                        |
|------------------------------------------|------------------------------------------|----------------------------------|
| Halogen compounds (continued)            |                                          |                                  |
| Dibromoethane                            | C                                        | -1.48                            |
| meso-2,3-Dibromosuccinic acid            | Acetate buffer, pH 4.0                   | -0.23, -0.89                     |
| Dichlorobenzenes                         | C                                        | -2.5                             |
| Dichloromethane                          | C                                        | -1.60                            |
| Diiodomethane                            | C                                        | -1.12, -1.53                     |
| Hexabromobenzene                         | C                                        | -0.8, -1.5                       |
| Hexachlorobenzene                        | C                                        | -1.4, -1.7                       |
| Iodobenzene                              | A                                        | -1.72                            |
| Iodoethane                               | C                                        | -1.67                            |
| Iodomethane                              | A                                        | -2.12                            |
|                                          | C                                        | -1.63                            |
| Tetrabromomethane                        | C                                        | -0.3, -0.75, -1.49               |
| Tetraiodomethane                         | C                                        | -0.45, -1.05, -1.46              |
| Tribromomethane                          | C                                        | -0.64, -1.47                     |
| $\alpha,\alpha,\alpha$ -Trichlorotoluene | C                                        | -0.68, -1.65, -2.00              |
| Nitro and nitroso compounds              |                                          |                                  |
| 1,2-Dinitrobenzene                       | Phthalate buffer, pH 2.5                 | -0.12, -0.32, -1.26              |
|                                          | Borate buffer, pH 9.2                    | -0.38, -0.74                     |
| 1,3-Dinitrobenzene                       | Phthalate buffer, pH 2.5                 | -0.17, -0.29                     |
|                                          | Borate buffer, pH 9.2                    | -0.46, -0.68                     |
| 1,4-Dinitrobenzene                       | Phthalate buffer, pH 2.5                 | -0.12, -0.33                     |
|                                          | Borate buffer, pH 9.2                    | -0.35, -0.80                     |
| Methyl nitrobenzoates                    | Buffer+10% EtOH, pH 2.0                  | -0.20 to -0.25<br>-0.68 to -0.74 |
| <i>p</i> -Nitroacetophenone              | Britton-Robinson buffer, pH 2.2          | -0.16, -0.61, -1.09              |
|                                          | Britton-Robinson buffer, pH 10.0         | -0.51, -1.40, -1.73              |
| <i>o</i> -Nitroaniline                   | 0.03 M LiCl+0.02 M benzoic acid in EtOH  | -0.88                            |
| <i>m</i> -Nitroaniline                   | Britton-Robinson buffer, pH 4.3          | -0.3, -0.8                       |
|                                          | Britton-Robinson buffer, pH 7.2          | -0.5                             |
|                                          | Britton-Robinson buffer, pH 9.2          | -0.7                             |
| <i>p</i> -Nitroaniline                   | pH 2.0                                   | -0.36                            |
|                                          | Acetate buffer, pH 4.6                   | -0.5                             |
| <i>o</i> -Nitroanisole                   | Buffer+10% EtOH, pH 2.0                  | -0.29, -0.58                     |
| <i>p</i> -Nitroanisole                   | Buffer+10% EtOH, pH 2.0                  | -0.35, -0.64                     |
| 1-Nitroanthraquinone                     | Britton-Robinson buffer, pH 7.0          | -0.16                            |
| Nitrobenzene                             | HCl+KCl+8% EtOH, pH 0.5                  | -0.16, -0.76                     |
|                                          | Phthalate buffer, pH 2.5                 | -0.30                            |
|                                          | Borate buffer, pH 9.2                    | -0.70                            |
| Nitroresols                              | Britton-Robinson buffer, pH 2.2          | -0.2 to -0.3                     |
|                                          | Britton-Robinson buffer, pH 4.5          | -0.4 to -0.5                     |
|                                          | Britton-Robinson buffer, pH 8.0          | -0.6                             |
| Nitroethane                              | Britton-Robinson buffer+30% MeOH, pH 1.8 | -0.7                             |
|                                          | Britton-Robinson buffer+30% MeOH, pH 4.6 | -0.8                             |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                                | Solvent system                            | $E_{1/2}$    |
|-----------------------------------------|-------------------------------------------|--------------|
| Nitro and nitroso compounds (continued) |                                           |              |
| 2-Nitrohydroquinone                     | Phosphate buffer+citrate buffer, pH 2.1   | -0.2         |
|                                         | Phosphate buffer+citrate buffer, pH 5.2   | -0.4         |
|                                         | Phosphate buffer+citrate buffer, pH 8.0   | -0.5         |
| Nitromethane                            | Britton-Robinson buffer+30% MeOH, pH 1.8  | -0.8         |
|                                         | Britton-Robinson buffer+30% MeOH, pH 4.6  | -0.85        |
| o-Nitrophenol                           | Britton-Robinson buffer+10% EtOH, pH 2.0  | -0.23        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 4.0  | -0.4         |
|                                         | Britton-Robinson buffer+10% EtOH, pH 8.0  | -0.65        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 10.0 | -0.80        |
| m-Nitrophenol                           | Britton-Robinson buffer+10% EtOH, pH 2.0  | -0.37        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 4.0  | -0.40        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 8.0  | -0.64        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 10.0 | -0.76        |
| p-Nitrophenol                           | Britton-Robinson buffer+10% EtOH, pH 2.0  | -0.35        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 4.0  | -0.50        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 8.0  | -0.82        |
|                                         | Britton-Robinson buffer+10% EtOH, pH 10.0 | -0.82        |
| 1-Nitropropane                          | Britton-Robinson buffer+30% MeOH, pH 1.8  | -0.73        |
|                                         | Britton-Robinson buffer+30% MeOH, pH 8.6  | -0.88        |
|                                         | Britton-Robinson buffer+30% MeOH, pH 8.0  | -0.95        |
|                                         | McIlvaine buffer, pH 2.1                  | -0.53        |
| 2-Nitropropane                          | McIlvaine buffer, pH 5.1                  | -0.81        |
|                                         | McIlvaine buffer, pH 6.0                  | -0.03        |
| Nitrosobenzene                          | McIlvaine buffer, pH 8.0                  | -0.14        |
|                                         | D+buffer, pH 4.0                          | +0.02        |
| 1-Nitroso-2-naphthol                    | D+buffer, pH 7.0                          | -0.20        |
|                                         | D+buffer, pH 9.0                          | -0.31        |
|                                         | pH 2.0                                    | -0.84        |
| N-Nitrosophenylhydroxylamine            | Phthalate buffer, pH 2.5                  | -0.35, -0.66 |
| o-Nitrotoluene                          | Phthalate buffer, pH 7.4                  | -0.60, -1.06 |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(Continued)

| Compound                                             | Solvent system                                                     | $E_{1/2}$                                        |
|------------------------------------------------------|--------------------------------------------------------------------|--------------------------------------------------|
| Nitro and nitroso compounds (continued)              |                                                                    |                                                  |
| <i>m</i> -Nitrotoluene (also <i>p</i> -nitrotoluene) | Phthalate buffer, pH 2.5<br>Phthalate buffer, pH 7.4               | − 0.30, − 0.53<br>− 0.58, − 1.06                 |
| Tetranitromethane                                    | pH 12.0                                                            | − 0.41                                           |
| 1,3,5-Trinitrobenzene                                | Phthalate buffer, pH 4.1<br>Borate buffer, pH 9.2                  | − 0.20, − 0.29, − 0.34<br>− 0.34, − 0.48, − 0.65 |
| Heterocyclic compounds containing nitrogen           |                                                                    |                                                  |
| Acridine                                             | D, pH 8.3                                                          | − 0.80, − 1.45                                   |
| Cinchonine                                           | B, pH 3                                                            | − 0.90                                           |
| 2-Furanmethanol                                      | Britton-Robinson buffer, pH 2.0<br>Britton-Robinson buffer, pH 5.8 | − 0.96<br>− 1.38, − 1.70                         |
| 2-Hydroxyphenazine                                   | Britton-Robinson buffer, pH 4.0                                    | − 0.24                                           |
| 8-Hydroxyquinoline                                   | B, pH 5.0<br>Phosphate buffer, pH 8.0                              | − 1.12<br>− 1.18, − 1.71                         |
| 3-Methylpyridine                                     | D+0.1 <i>M</i> LiCl                                                | − 1.76                                           |
| 4-Methylpyridine                                     | D+0.1 <i>M</i> LiCl                                                | − 1.87                                           |
| Phenazine                                            | Phosphate buffer+citrate buffer,<br>pH 7.0                         | − 0.36                                           |
| Pyridine                                             | Phosphate buffer+citrate buffer,<br>pH 7.0                         | − 1.75                                           |
| Pyridine-2-carboxylic acid                           | B, pH 4.1                                                          | − 1.10                                           |
|                                                      | B, pH 9.3                                                          | − 1.48, − 1.94                                   |
| Pyridine-3-carboxylic acid                           | 0.1 <i>M</i> HCl                                                   | − 1.08                                           |
| Pyridine-4-carboxylic acid                           | Britton-Robinson buffer, pH 6.1                                    | − 1.14                                           |
|                                                      | pH 9.0                                                             | − 1.39, − 1.68                                   |
| Pyrimidine                                           | Citrate buffer, pH 3.6<br>Ammonia buffer, pH 9.2                   | − 0.92, − 1.24<br>− 1.54                         |
| Quinoline-8-carboxylic acid                          | pH 9                                                               | − 1.11                                           |
| Quinoxaline                                          | Phosphate buffer+citrate buffer,<br>pH 7.0                         | − 0.66, − 1.52                                   |
| Azo, hydrazine, hydroxylamine, and oxime compounds   |                                                                    |                                                  |
| Azobenzene                                           | D, pH 4.0                                                          | − 0.20                                           |
|                                                      | D, pH 7.0                                                          | − 0.50                                           |
| Azoxybenzene                                         | Buffer+20% EtOH, pH 6.3                                            | − 0.30                                           |
| Benzoin 1-oxime                                      | Buffer, pH 2.0                                                     | − 0.88                                           |
|                                                      | Buffer, pH 5.6                                                     | − 1.08                                           |
|                                                      | Buffer, pH 8.2                                                     | − 1.67                                           |
| Benzoylhydrazine                                     | 0.13 <i>M</i> NaOH, pH 13.0                                        | − 0.30                                           |
| Dimethylglyoxime                                     | Ammonia buffer, pH 9.6                                             | − 1.63                                           |
| Hydrazine                                            | Britton-Robinson buffer, pH 9.3                                    | − 0.09                                           |
| Hydroxylamine                                        | Britton-Robinson buffer, pH 4.6<br>Britton-Robinson buffer, pH 9.2 | − 1.42<br>− 1.65                                 |

**TABLE 8.31** Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C  
(*Continued*)

| Compound                                                                | Solvent system                      | $E_{1/2}$          |
|-------------------------------------------------------------------------|-------------------------------------|--------------------|
| Azo, hydrazine, hydroxylamine, and oxime compounds ( <i>continued</i> ) |                                     |                    |
| Oxamide                                                                 | Acetate buffer                      | − 1.55             |
| Phenylhydrazine                                                         | McIlvaine buffer, pH 2              | + 0.19             |
|                                                                         | 0.13 M NaOH, pH 13.0                | − 0.36             |
| Phenylhydroxylamine                                                     | McIlvaine buffer + 10% EtOH, pH 2   | − 0.68             |
|                                                                         | McIlvaine buffer + 10 EtOH, pH 4–10 | − 0.33<br>0.061 pH |
| Salicylaldoxime                                                         | Phosphate buffer, pH 5.4            | − 1.02             |
| Thiosemicarbazide                                                       | Borate buffer, pH 9.3               | − 0.26             |
| Thiourea                                                                | 0.1 M sulfuric acid                 | + 0.02             |
| Indicators and dyestuffs                                                |                                     |                    |
| Brilliant Green                                                         | HCl + KCl, pH 2.0                   | − 0.2, − 0.5       |
| Indigo carmine                                                          | pH 2.5                              | − 0.24             |
| Indigo disulfonate                                                      | pH 7.0                              | − 0.37             |
| Malachite Green G                                                       | HCl + KCl, pH 2.0                   | − 0.2, − 0.5       |
| Metanil yellow                                                          | Phosphate buffer + 1% EtOH, pH 7.0  | − 0.51             |
| Methylene blue                                                          | Britton-Robinson buffer, pH 4.9     | − 0.15             |
|                                                                         | Britton-Robinson buffer, pH 9.2     | − 0.30             |
| Methylene green                                                         | Phosphate buffer + 1% EtOH, pH 7.0  | − 0.12             |
| Methyl orange                                                           | Phosphate buffer + 1% EtOH, pH 7.0  | − 0.51             |
| Morin                                                                   | D, pH 7.6                           | − 1.7              |
| Neutral red                                                             | Britton-Robinson buffer, pH 2.0     | − 0.21             |
|                                                                         | Britton-Robinson buffer, pH 7.0     | − 0.57             |
| Peroxide                                                                |                                     |                    |
| Ethyl peroxide                                                          | 0.02 M HCl                          | − 0.2              |

## 8.7 CONDUCTANCE

**TABLE 8.32** Limiting Equivalent Ionic Conductances in Aqueous Solutions

In  $10^{-4} \text{ m}^2 \cdot \text{S} \cdot \text{equiv}^{-1}$  or  $\text{mho} \cdot \text{cm}^2 \cdot \text{equiv}^{-1}$ .

| Ion                                                          | Temperature, °C |       |       |
|--------------------------------------------------------------|-----------------|-------|-------|
|                                                              | 0               | 18    | 25    |
| <b>Inorganic cations</b>                                     |                 |       |       |
| Ag <sup>+</sup>                                              | 33              | 54.5  | 61.9  |
| Al <sup>3+</sup>                                             | 29              |       | 61    |
| Ba <sup>2+</sup>                                             | 33.6            | 54.3  | 63.9  |
| Be <sup>2+</sup>                                             |                 |       | 45    |
| Ca <sup>2+</sup>                                             | 30.8            | 51    | 59.5  |
| Cd <sup>2+</sup>                                             | 28              | 45.1  | 54    |
| Ce <sup>3+</sup>                                             |                 |       | 70    |
| Co <sup>2+</sup>                                             | 28              | 45    | 53    |
| Co(NH <sub>3</sub> ) <sub>6</sub> <sup>3+</sup>              |                 |       | 100   |
| Co(ethylenediamine) <sub>3</sub> <sup>3+</sup>               |                 |       | 74.7  |
| Cr <sup>3+</sup>                                             |                 |       | 67    |
| Cs <sup>+</sup>                                              | 44              | 68    | 77.3  |
| Cu <sup>2+</sup>                                             | 28              | 45.3  | 56.6  |
| D <sup>+</sup> (deuterium)                                   |                 | 213.7 |       |
| Dy <sup>3+</sup>                                             |                 |       | 65.7  |
| Er <sup>3+</sup>                                             |                 |       | 66.0  |
| Eu <sup>3+</sup>                                             |                 |       | 67.9  |
| Fe <sup>2+</sup>                                             | 28              | 45.3  | 53.5  |
| Fe <sup>3+</sup>                                             |                 |       | 69    |
| Gd <sup>3+</sup>                                             |                 |       | 67.4  |
| H <sup>+</sup>                                               | 224.1           | 315.8 | 350.1 |
| Hg <sub>2</sub> <sup>2+</sup>                                |                 |       | 68.7  |
| Hg <sup>2+</sup>                                             |                 |       | 63.6  |
| Ho <sup>3+</sup>                                             |                 |       | 66.3  |
| K <sup>+</sup>                                               | 40.3            | 64.6  | 73.5  |
| La <sup>3+</sup>                                             | 35.0            | 59.2  | 69.6  |
| Li <sup>+</sup>                                              | 19.1            | 33.4  | 38.69 |
| Mg <sup>2+</sup>                                             | 28.5            | 46    | 53.06 |
| Mn <sup>2+</sup>                                             | 27              | 44.5  | 53.5  |
| NH <sub>4</sub> <sup>+</sup>                                 | 40.3            | 64    | 73.7  |
| N <sub>2</sub> H <sub>5</sub> <sup>+</sup> (hydrazinium 1 +) |                 |       | 59    |
| Na <sup>+</sup>                                              | 25.85           | 43.5  | 50.11 |
| Nd <sup>3+</sup>                                             |                 |       | 69.6  |
| Ni <sup>2+</sup>                                             | 28              | 45    | 50    |
| Pb <sup>2+</sup>                                             | 37.5            | 60.5  | 71    |
| Pr <sup>3+</sup>                                             |                 |       | 69.6  |
| Ra <sup>2+</sup>                                             | 33              | 56.6  | 66.8  |
| Rb <sup>+</sup>                                              | 43.5            | 67.5  | 77.8  |
| Sc <sup>3+</sup>                                             |                 |       | 64.7  |
| Sm <sup>3+</sup>                                             |                 |       | 68.5  |
| Sr <sup>2+</sup>                                             | 31              | 51    | 59.46 |
| Tl <sup>+</sup>                                              | 43.3            | 66    | 74.9  |
| Tm <sup>3+</sup>                                             |                 |       | 65.5  |
| UO <sub>2</sub> <sup>2+</sup>                                |                 |       | 32    |
| Y <sup>3+</sup>                                              |                 |       | 62    |
| Yb <sup>3+</sup>                                             |                 |       | 65.2  |
| Zn <sup>2+</sup>                                             | 28              | 45.0  | 52.8  |

TABLE 8.32 Limiting Equivalent Ionic Conductances in Aqueous Solutions (Continued)

| Ion                                                         | Temperature, °C |       |       |
|-------------------------------------------------------------|-----------------|-------|-------|
|                                                             | 0               | 18    | 25    |
| <b>Inorganic anions</b>                                     |                 |       |       |
| Au(CN) <sub>2</sub> <sup>-</sup>                            |                 |       | 50    |
| Au(CN) <sub>4</sub> <sup>-</sup>                            |                 |       | 36    |
| B(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> <sup>-</sup> |                 |       | 21    |
| Br <sup>-</sup>                                             | 43.1            | 67.6  | 78.1  |
| Br <sub>3</sub> <sup>-</sup>                                |                 |       | 43    |
| BrO <sub>3</sub> <sup>-</sup>                               | 31.0            | 49.0  | 55.7  |
| Cl <sup>-</sup>                                             | 41.4            | 65.5  | 76.31 |
| ClO <sub>2</sub> <sup>-</sup>                               |                 |       | 52    |
| ClO <sub>3</sub> <sup>-</sup>                               | 36              | 55.0  | 64.6  |
| ClO <sub>4</sub> <sup>-</sup>                               | 37.3            | 59.1  | 67.3  |
| CN <sup>-</sup>                                             |                 |       | 78    |
| CO <sub>3</sub> <sup>2+</sup>                               | 36              | 60.5  | 69.3  |
| Co(CN) <sub>6</sub> <sup>3-</sup>                           |                 |       | 98.9  |
| CrO <sub>4</sub> <sup>2-</sup>                              | 42              | 72    | 85    |
| F <sup>-</sup>                                              |                 | 46.6  | 55.4  |
| Fe(CN) <sub>6</sub> <sup>4-</sup>                           |                 |       | 110.4 |
| Fe(CN) <sub>6</sub> <sup>3-</sup>                           |                 |       | 100.9 |
| H <sub>2</sub> AsO <sub>4</sub> <sup>-</sup>                |                 |       | 34    |
| HCO <sub>3</sub> <sup>-</sup>                               |                 |       | 44.5  |
| HF <sub>2</sub> <sup>-</sup>                                |                 |       | 75    |
| HPO <sub>4</sub> <sup>2-</sup>                              |                 |       | 33    |
| H <sub>2</sub> PO <sub>4</sub> <sup>-</sup>                 |                 | 28    | 33    |
| HS <sup>-</sup>                                             | 40              | 57    | 65    |
| HSO <sub>3</sub> <sup>-</sup>                               | 27              |       | 50    |
| HSO <sub>4</sub> <sup>-</sup>                               |                 |       | 50    |
| H <sub>2</sub> SbO <sub>4</sub> <sup>-</sup>                |                 |       | 31    |
| I <sup>-</sup>                                              | 42.0            | 66.5  | 76.9  |
| IO <sub>3</sub> <sup>-</sup>                                | 21.0            | 33.9  | 40.5  |
| IO <sub>4</sub> <sup>-</sup>                                |                 | 49    | 54.5  |
| MnO <sub>4</sub> <sup>-</sup>                               | 36              | 53    | 61.3  |
| MoO <sub>4</sub> <sup>2-</sup>                              |                 |       | 74.5  |
| N <sub>3</sub> <sup>-</sup>                                 |                 |       | 69.5  |
| N(CN) <sub>2</sub> <sup>-</sup>                             |                 |       | 54.5  |
| NO <sub>2</sub> <sup>-</sup>                                | 44              | 59    | 71.8  |
| NO <sub>3</sub> <sup>-</sup>                                | 40.2            | 61.7  | 71.42 |
| NH <sub>2</sub> SO <sub>3</sub> <sup>-</sup> (sulfamate)    |                 |       | 48.6  |
| OCN <sup>-</sup> (cyanate)                                  |                 | 54.8  | 64.6  |
| OH <sup>-</sup>                                             | 117.8           | 175.8 | 198   |
| PF <sub>6</sub> <sup>-</sup>                                |                 |       | 56.9  |
| PO <sub>3</sub> F <sup>2-</sup>                             |                 |       | 63.3  |
| PO <sub>4</sub> <sup>3-</sup>                               |                 |       | 69.0  |
| P <sub>2</sub> O <sub>7</sub> <sup>4-</sup>                 |                 |       | 96    |
| P <sub>3</sub> O <sub>9</sub> <sup>3-</sup>                 |                 |       | 83.6  |
| P <sub>3</sub> O <sub>10</sub> <sup>5-</sup>                |                 |       | 109   |
| ReO <sub>4</sub> <sup>-</sup>                               |                 | 46.5  | 54.9  |
| SCN <sup>-</sup> (thiocyanate)                              | 41.7            | 56.6  | 66.5  |
| SeCN <sup>-</sup>                                           |                 |       | 64.7  |
| SeO <sub>4</sub> <sup>2-</sup>                              |                 | 65    | 75.7  |
| SO <sub>3</sub> <sup>-</sup>                                |                 |       | 79.9  |

**TABLE 8.32** Limiting Equivalent Ionic Conductances in Aqueous Solutions (*Continued*)

| Ion                                          | Temperature, °C |      |      |
|----------------------------------------------|-----------------|------|------|
|                                              | 0               | 18   | 25   |
| $\text{SO}_4^{2-}$                           | 41              | 68.3 | 80.0 |
| $\text{S}_2\text{O}_3^{2-}$                  |                 |      | 85.0 |
| $\text{S}_2\text{O}_4^{2-}$                  | 34              |      | 66.5 |
| $\text{S}_2\text{O}_6^{2-}$                  |                 |      | 93   |
| $\text{S}_2\text{O}_8^{2-}$                  |                 |      | 86   |
| $\text{WO}_4^{2-}$                           | 35              | 59   | 69.4 |
| <b>Organic cations</b>                       |                 |      |      |
| Decylpyridinium <sup>+</sup>                 |                 |      | 29.5 |
| Diethylammonium <sup>+</sup>                 |                 |      | 42.0 |
| Dimethylammonium <sup>+</sup>                |                 |      | 51.5 |
| Dipropylammonium <sup>+</sup>                |                 |      | 30.1 |
| Dodecylammonium <sup>+</sup>                 |                 |      | 23.8 |
| Ethylammonium <sup>+</sup>                   |                 |      | 47.2 |
| Ethyltrimethylammonium <sup>+</sup>          |                 |      | 40.5 |
| Isobutylammonium <sup>+</sup>                |                 |      | 38.0 |
| Methylammonium <sup>+</sup>                  |                 |      | 58.3 |
| Piperidinium <sup>+</sup>                    |                 |      | 37.2 |
| Propylammonium <sup>+</sup>                  |                 |      | 40.8 |
| Tetrabutylammonium <sup>+</sup>              |                 |      | 19.5 |
| Tetraethylammonium <sup>+</sup>              |                 |      | 32.6 |
| Tetramethylammonium <sup>+</sup>             |                 |      | 44.9 |
| Tetrapropylammonium <sup>+</sup>             |                 |      | 23.5 |
| Triethylsulfonium <sup>+</sup>               |                 |      | 36.1 |
| Trimethylammonium <sup>+</sup>               |                 |      | 47.2 |
| Trimethylsulfonium <sup>+</sup>              |                 |      | 51.4 |
| Tripropylammonium <sup>+</sup>               |                 |      | 26.1 |
| <b>Organic anions</b>                        |                 |      |      |
| Acetate <sup>-</sup>                         | 20              | 34   | 41   |
| Benzoate <sup>-</sup>                        |                 |      | 32.4 |
| Bromoacetate <sup>-</sup>                    |                 |      | 39.2 |
| Bromobenzoate <sup>-</sup>                   |                 |      | 30   |
| Butanoate <sup>-</sup>                       |                 |      | 32.6 |
| Chloroacetate <sup>-</sup>                   |                 |      | 42.2 |
| <i>m</i> -Chlorobenzoate <sup>-</sup>        |                 |      | 31   |
| <i>o</i> -Chlorobenzoate <sup>-</sup>        |                 |      | 30.5 |
| Citrate(3 <sup>-</sup> )                     |                 |      | 70.2 |
| Crotonate <sup>-</sup>                       |                 |      | 33.2 |
| Cyanoacetate <sup>-</sup>                    |                 |      | 43.4 |
| Cyclohexanecarboxylate <sup>-</sup>          |                 |      | 28.7 |
| Cyclopropane-1,3-dicarboxylate <sup>2-</sup> |                 |      | 53.4 |
| Decylsulfonate <sup>-</sup>                  |                 |      | 26   |
| Dichloroacetate <sup>-</sup>                 |                 |      | 38.3 |
| Diethylbarbiturate(2 <sup>-</sup> )          |                 |      | 26.3 |
| Dihydrogencitrate <sup>-</sup>               |                 |      | 30   |
| Dimethylmalonate(2 <sup>-</sup> )            |                 |      | 49.4 |
| 3,5-Dinitrobenzoate <sup>-</sup>             |                 |      | 28.3 |
| Dodecylsulfonate <sup>-</sup>                |                 |      | 24   |
| Ethylmalonate <sup>-</sup>                   |                 |      | 49.3 |
| Ethylsulfonate <sup>-</sup>                  |                 |      | 39.6 |



**TABLE 8.32** Limiting Equivalent Ionic Conductances in Aqueous Solutions (*Continued*)

| Ion                                  | Temperature, °C |    |       |
|--------------------------------------|-----------------|----|-------|
|                                      | 0               | 18 | 25    |
| Fluoroacetate <sup>−</sup>           |                 |    | 44.4  |
| Fluorobenzoate <sup>−</sup>          |                 |    | 33    |
| Formate <sup>−</sup>                 |                 | 47 | 54.6  |
| Fumarate(2 <sup>−</sup> )            |                 |    | 61.8  |
| Glutarate(2 <sup>−</sup> )           |                 |    | 52.6  |
| Hydrogenoxalate (1 <sup>−</sup> )    |                 |    | 40.2  |
| Iodoacetate <sup>−</sup>             |                 |    | 40.6  |
| Lactate(1 <sup>−</sup> )             |                 |    | 38.8  |
| Malate(2 <sup>−</sup> )              |                 |    | 58.8  |
| Malonate(1 <sup>−</sup> )            |                 |    | 63.5  |
| 3-Methylbutanoate <sup>−</sup>       |                 |    | 32.7  |
| Methylsulfonate <sup>−</sup>         |                 |    | 48.8  |
| Naphthylacetate <sup>−</sup>         |                 |    | 28.4  |
| 1,8-Octanedioate(2 <sup>−</sup> )    |                 |    | 36    |
| Octylsulfonate <sup>−</sup>          |                 |    | 29    |
| Oxalate(2 <sup>−</sup> )             |                 |    | 74.11 |
| Phenylacetate <sup>−</sup>           |                 |    | 30.6  |
| <i>m</i> -Phthalate(2 <sup>−</sup> ) |                 |    | 54.7  |
| <i>o</i> -Phthalate(2 <sup>−</sup> ) |                 |    | 52.3  |
| Picrate <sup>−</sup>                 |                 |    | 30.37 |
| Propanoate <sup>−</sup>              |                 |    | 35.8  |
| Propylsulfonate <sup>−</sup>         |                 |    | 37.1  |
| Salicylate <sup>−</sup>              |                 |    | 36    |
| Succinate(2 <sup>−</sup> )           |                 |    | 58.8  |
| Tartrate(2 <sup>−</sup> )            |                 | 55 | 59.6  |
| Trichloroacetate <sup>−</sup>        |                 |    | 36.6  |
| Trimethylacetate <sup>−</sup>        |                 |    | 31.9  |

**TABLE 8.33** Standard Solutions for Calibrating Conductivity Vessels

The values of conductivity  $\kappa$  are corrected for the conductivity of the water used. The cell constant  $\theta$  of a conductivity cell can be obtained from the equation

$$\theta = \frac{\kappa R R_{\text{solv}}}{R_{\text{solv}} - R}$$

where  $R$  is the resistance measured when the cell is filled with a solution of the composition stated in the table below, and  $R_{\text{solv}}$  is the resistance when the cell is filled with solvent at the same temperature.

| Grams KCl per Kilogram<br>Solution (in vacuo) | Conductivity in $\text{ohm}^{-1} \cdot \text{cm}^{-1}$ at |                          |                          |
|-----------------------------------------------|-----------------------------------------------------------|--------------------------|--------------------------|
|                                               | 0°C                                                       | 18°C                     | 25°C                     |
| 71.135 2                                      | 0.065 14 <sub>4</sub>                                     | 0.097 79 <sub>0</sub>    | 0.111 28 <sub>7</sub>    |
| 7.419 13                                      | 0.007 134 <sub>4</sub>                                    | 0.011 161 <sub>2</sub>   | 0.012 849 <sub>7</sub>   |
| 0.745 263*                                    | 0.000 773 2 <sub>6</sub>                                  | 0.001 219 9 <sub>2</sub> | 0.001 408 0 <sub>8</sub> |

\* Virtually 0.0100 *M*.

From the data of Jones and Bradshaw, *J. Am. Chem. Soc.*, **55**, 1780 (1933). The original data have been converted from (int. ohm)<sup>−1</sup> cm<sup>−1</sup>.

**TABLE 8.34** Electrical Conductivity of Various Pure Liquids

| Liquid               | Temp.<br>°C | mhos/cm<br>or $\text{ohm}^{-1} \cdot \text{cm}^{-1}$ | Liquid               | Temp.<br>°C | mhos/cm<br>or $\text{ohm}^{-1} \cdot \text{cm}^{-1}$ |
|----------------------|-------------|------------------------------------------------------|----------------------|-------------|------------------------------------------------------|
| Acetaldehyde         | 15          | $1.7 \times 10^{-6}$                                 | Epichlorohydrin      | 25          | $3.4 \times 10^{-8}$                                 |
| Acetamide            | 100         | $< 4.3 \times 10^{-5}$                               | Ethyl acetate        | 25          | $< 1 \times 10^{-9}$                                 |
| Acetic acid          | 0           | $5 \times 10^{-9}$                                   | Ethyl acetoacetate   | 25          | $4 \times 10^{-8}$                                   |
|                      | 25          | $1.12 \times 10^{-8}$                                | Ethyl alcohol        | 25          | $1.35 \times 10^{-9}$                                |
| Acetic anhydride     | 0           | $1 \times 10^{-6}$                                   | Ethylamine           | 0           | $4 \times 10^{-7}$                                   |
|                      | 25          | $4.8 \times 10^{-7}$                                 | Ethyl benzoate       | 25          | $< 1 \times 10^{-9}$                                 |
| Acetone              | 18          | $2 \times 10^{-8}$                                   | Ethyl bromide        | 25          | $< 2 \times 10^{-8}$                                 |
|                      | 25          | $6 \times 10^{-8}$                                   | Ethylene bromide     | 19          | $< 2 \times 10^{-10}$                                |
| Acetonitrile         | 20          | $7 \times 10^{-6}$                                   | Ethylene chloride    | 25          | $3 \times 10^{-8}$                                   |
| Acetophenone         | 25          | $6 \times 10^{-9}$                                   | Ethyl ether          | 25          | $< 4 \times 10^{-13}$                                |
| Acetyl bromide       | 25          | $2.4 \times 10^{-6}$                                 | Ethylidene chloride  | 25          | $< 1.7 \times 10^{-8}$                               |
| Acetyl chloride      | 25          | $4 \times 10^{-7}$                                   | Ethyl iodide         | 25          | $< 2 \times 10^{-8}$                                 |
| Alizarin             | 233         | $1.45 \times 10^{-6} (?)$                            | Ethyl isothiocyanate | 25          | $1.26 \times 10^{-7}$                                |
| Allyl alcohol        | 25          | $7 \times 10^{-6}$                                   | Ethyl nitrate        | 25          | $5.3 \times 10^{-7}$                                 |
| Ammonia              | -79         | $1.3 \times 10^{-7}$                                 | Ethyl thiocyanate    | 25          | $1.2 \times 10^{-6}$                                 |
| Aniline              | 25          | $2.4 \times 10^{-8}$                                 | Eugenol              | 25          | $< 1.7 \times 10^{-8}$                               |
| Anthracene           | 230         | $3 \times 10^{-10}$                                  |                      |             |                                                      |
| Arsenic tribromide   | 35          | $1.5 \times 10^{-6}$                                 | Formamide            | 25          | $4 \times 10^{-6}$                                   |
| Arsenic trichloride  | 25          | $1.2 \times 10^{-6}$                                 | Formic acid          | 18          | $5.6 \times 10^{-5}$                                 |
|                      |             |                                                      |                      | 25          | $6.4 \times 10^{-5}$                                 |
| Benzaldehyde         | 25          | $1.5 \times 10^{-7}$                                 | Furfural             | 25          | $1.5 \times 10^{-6}$                                 |
| Benzene              | ...         | $7.6 \times 10^{-8}$                                 |                      |             |                                                      |
| Benzoic acid         | 125         | $3 \times 10^{-9}$                                   | Gallium              | 30          | 36,800                                               |
| Benzonitrile         | 25          | $5 \times 10^{-8}$                                   | Glycerol             | 25          | $6.4 \times 10^{-8}$                                 |
| Benzyl alcohol       | 25          | $1.8 \times 10^{-6}$                                 | Glycol               | 25          | $3 \times 10^{-7}$                                   |
| Benzylamine          | 25          | $< 1.7 \times 10^{-8}$                               | Guaiacol             | 25          | $2.8 \times 10^{-7}$                                 |
| Benzyl benzoate      | 25          | $< 1 \times 10^{-9}$                                 |                      |             |                                                      |
| Bromine              | 17.2        | $1.3 \times 10^{-13}$                                | Heptane              | ...         | $< 1 \times 10^{-13}$                                |
| Bromobenzene         | 25          | $< 2 \times 10^{-11}$                                | Hexane               | 18          | $< 1 \times 10^{-18}$                                |
| Bromoform            | 25          | $< 2 \times 10^{-8}$                                 | Hydrogen bromide     | -80         | $8 \times 10^{-9}$                                   |
| iso-Butyl alcohol    | 25          | $8 \times 10^{-8}$                                   | Hydrogen chloride    | -96         | $1 \times 10^{-8}$                                   |
|                      |             |                                                      | Hydrogen cyanide     | 0           | $3.3 \times 10^{-6}$                                 |
| Capronitrile         | 25          | $3.7 \times 10^{-6}$                                 | Hydrogen iodide      | B.P.        | $2 \times 10^{-7}$                                   |
| Carbon disulfide     | 1           | $7.8 \times 10^{-18}$                                | Hydrogen sulfide     | B.P.        | $1 \times 10^{-11}$                                  |
| Carbon tetrachloride | 18          | $4 \times 10^{-18}$                                  |                      |             |                                                      |
| Chlorine             | -70         | $< 1 \times 10^{-16}$                                | Iodine               | 110         | $1.3 \times 10^{-10}$                                |
| Chloroacetic acid    | 60          | $1.4 \times 10^{-6}$                                 |                      |             |                                                      |
| m-Chloroaniline      | 25          | $5 \times 10^{-8}$                                   | Kerosene             | 25          | $< 1.7 \times 10^{-8}$                               |
| Chloroform           | 25          | $< 2 \times 10^{-8}$                                 |                      |             |                                                      |
| Chlorohydrin         | 25          | $5 \times 10^{-7}$                                   | Mercury              | 0           | 10,629.6                                             |
| m-Cresol             | 25          | $< 1.7 \times 10^{-8}$                               | Methyl acetate       | 25          | $3.4 \times 10^{-6}$                                 |
| Cyanogen             | ...         | $< 7 \times 10^{-9}$                                 | Methyl alcohol       | 18          | $4.4 \times 10^{-7}$                                 |
| Cymene               | 25          | $< 2 \times 10^{-8}$                                 | Methyl ethyl ketone  | 25          | $1 \times 10^{-7}$                                   |
|                      |             |                                                      | Methyl iodide        | 25          | $< 2 \times 10^{-8}$                                 |
| Dichloroacetic acid  | 25          | $7 \times 10^{-8}$                                   | Methyl nitrate       | 25          | $4.5 \times 10^{-6}$                                 |
| Dichlorohydrin       | 25          | $1.2 \times 10^{-5}$                                 | Methyl thiocyanate   | 25          | $1.5 \times 10^{-6}$                                 |
| Diethylamine         | -33.5       | $2.2 \times 10^{-9}$                                 |                      |             |                                                      |
| Diethyl carbonate    | 25          | $1.7 \times 10^{-8}$                                 | Naphthalene          | 82          | $4 \times 10^{-10}$                                  |
| Diethyl oxalate      | 25          | $7.6 \times 10^{-7}$                                 | Nitrobenzene         | 0           | $5 \times 10^{-9}$                                   |
| Diethyl sulfate      | 25          | $2.6 \times 10^{-7}$                                 | Nitromethane         | 18          | $6 \times 10^{-7}$                                   |
| Dimethyl sulfate     | 0           | $1.6 \times 10^{-7}$                                 | o- or m-Nitrotoluene | 25          | $< 2 \times 10^{-7}$                                 |
|                      |             |                                                      | Nonane               | 25          | $< 1.7 \times 10^{-8}$                               |

**TABLE 8.34** Electrical Conductivity of Various Pure Liquids (*Continued*)

| Liquid                     | Temp.<br>°C | mhos/cm<br>or ohm <sup>-1</sup> · cm <sup>-1</sup> | Liquid                                                | Temp.<br>°C | mhos/cm<br>or ohm <sup>-1</sup> · cm <sup>-1</sup> |
|----------------------------|-------------|----------------------------------------------------|-------------------------------------------------------|-------------|----------------------------------------------------|
| Oleic acid                 | 15          | <2 × 10 <sup>-10</sup>                             | Salicylaldehyde                                       | 25          | 1.6 × 10 <sup>-7</sup>                             |
| Pentane                    | 19.5        | <2 × 10 <sup>-10</sup>                             | Stearic acid                                          | 80          | <4 × 10 <sup>-13</sup>                             |
| Petroleum                  | ...         | 3 × 10 <sup>-13</sup>                              | Sulfonyl chloride,<br>SOCl <sub>2</sub>               | 25          | 2 × 10 <sup>-6</sup>                               |
| Phenetole                  | 25          | <1.7 × 10 <sup>-8</sup>                            | Sulfur                                                | 115         | 1 × 10 <sup>-12</sup>                              |
| Phenol                     | 25          | <1.7 × 10 <sup>-8</sup>                            |                                                       | 130         | 5 × 10 <sup>-12</sup>                              |
| Phenyl isothiocyanate      | 25          | 1.4 × 10 <sup>-6</sup>                             |                                                       | 440         | 1.2 × 10 <sup>-7</sup>                             |
| Phosgene                   | 25          | 7 × 10 <sup>-9</sup>                               | Sulfur dioxide                                        | 35          | 1.5 × 10 <sup>-8</sup>                             |
| Phosphorus                 | 25          | 4 × 10 <sup>-7</sup>                               | Sulfuric acid                                         | 25          | 1 × 10 <sup>-2</sup>                               |
| Phosphorus oxychloride     | 25          | 2.2 × 10 <sup>-6</sup>                             | Sulfuryl chloride,<br>SO <sub>2</sub> Cl <sub>2</sub> | 25          | 3 × 10 <sup>-8</sup>                               |
| Pinene                     | 23          | <2 × 10 <sup>-10</sup>                             |                                                       |             |                                                    |
| Piperidine                 | 25          | <2 × 10 <sup>-7</sup>                              | Toluene                                               | ...         | <1 × 10 <sup>-14</sup>                             |
| Propionaldehyde            | 25          | 8.5 × 10 <sup>-7</sup>                             | <i>o</i> -Toluidine                                   | 25          | <2 × 10 <sup>-6</sup>                              |
| Propionic acid             | 25          | <1 × 10 <sup>-9</sup>                              | <i>p</i> -Toluidine                                   | 100         | 6.2 × 10 <sup>-8</sup>                             |
| Propionitrile              | 25          | <1 × 10 <sup>-7</sup>                              | Trichloroacetic acid                                  | 25          | 3 × 10 <sup>-9</sup>                               |
| <i>n</i> -Propyl alcohol   | 18          | 5 × 10 <sup>-8</sup>                               | Trimethylamine                                        | -33.5       | 2.2 × 10 <sup>-10</sup>                            |
|                            | 25          | 2 × 10 <sup>-8</sup>                               | Turpentine                                            | ...         | 2 × 10 <sup>-13</sup>                              |
| <i>iso</i> -Propyl alcohol | 25          | 3.5 × 10 <sup>-6</sup>                             | <i>iso</i> -Valeric acid                              | 80          | <4 × 10 <sup>-13</sup>                             |
| <i>n</i> -Propyl bromide   | 25          | <2 × 10 <sup>-8</sup>                              |                                                       |             |                                                    |
| Pyridine                   | 18          | 5.3 × 10 <sup>-8</sup>                             | Water                                                 | 18          | 4 × 10 <sup>-8</sup>                               |
| Quinoline                  | 25          | 2.2 × 10 <sup>-8</sup>                             | Xylene                                                | ...         | <1 × 10 <sup>-15</sup>                             |

**TABLE 8.35** Equivalent Conductivities of Electrolytes in Aqueous Solutions at 18°C

The unit of  $\Lambda$  in the table is  $\Omega^{-1} \cdot \text{cm}^{-2} \cdot \text{equiv}^{-1}$ . The entities to which the equivalent relates are given in the first column.

| Electrolyte                                                          | Concentration, $N$ |       |       |      |      |      |      |      |      |      |      |
|----------------------------------------------------------------------|--------------------|-------|-------|------|------|------|------|------|------|------|------|
|                                                                      | 0.001              | 0.005 | 0.01  | 0.05 | 0.1  | 0.5  | 1.0  | 2.0  | 3.0  | 4.0  | 5.0  |
| Acetic acid                                                          | 41                 | 20.0  | 14.3  | 6.48 | 4.60 | 2.01 | 1.32 |      | 0.54 |      | 0.29 |
| AgNO <sub>3</sub>                                                    | 113.2              | 110.0 | 107.8 | 99.5 | 94.3 | 77.8 | 67.8 | 56.0 | 48.2 | 42.1 | 37.2 |
| ½Ag <sub>2</sub> SO <sub>4</sub>                                     | 116.3              | 108.4 | 102.9 |      |      |      |      |      |      |      |      |
| ⅓AlBr <sub>3</sub> (25°)                                             | 132                | 124   | 119   | 103  | 97   |      |      |      |      |      |      |
| ⅓AlCl <sub>3</sub>                                                   | 121.1              | 105.0 | 93.8  |      |      | 65.0 | 56.2 | 44.2 | 34.7 | 27.2 |      |
| ⅓AlI <sub>3</sub> (25°)                                              | 131                | 124   | 119   | 108  |      |      |      |      |      |      |      |
| ⅓Al(NO <sub>3</sub> ) <sub>3</sub> (25°)                             | 123                | 115   | 110   | 94   | 88   |      |      |      |      |      |      |
| ⅙Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> (25°)               | 107.2              | 76.8  | 60.6  |      |      |      |      |      |      |      |      |
| ½Ba(OAc) <sub>2</sub>                                                | 85.0               | 80.4  | 77.1  | 65.7 | 60.2 | 43.8 | 34.3 |      |      |      |      |
| ½Ba(BrO <sub>3</sub> ) <sub>2</sub> (25°)                            | 113.6              | 106.8 | 102.7 |      |      |      |      |      |      |      |      |
| ½BaCl <sub>2</sub>                                                   | 115.6              | 112.3 | 106.7 | 96.0 | 90.8 | 77.3 | 70.1 | 60.3 | 52.3 |      |      |
| ½Ba(NO <sub>3</sub> ) <sub>2</sub>                                   | 111.7              | 105.3 | 101.0 | 86.8 | 78.9 | 56.6 | 48.4 |      | 29.8 | 23.4 |      |
| ½Ba(OH) <sub>2</sub>                                                 | 216                | 213   | 207   | 191  | 180  |      |      |      |      |      |      |
| Butyric acid                                                         |                    |       |       |      |      | 1.66 | 0.98 | 0.46 | 0.26 | 0.18 | 0.11 |
| ½Ca(OAc) <sub>2</sub>                                                | 79.6               | 75.0  | 71.9  | 60.3 | 54.0 | 36.3 | 26.3 |      |      |      |      |
| ½CaCl <sub>2</sub>                                                   | 112.0              | 106.7 | 103.4 | 93.3 | 88.2 | 74.9 | 67.5 | 58.3 | 49.7 | 42.4 | 35.6 |
| ½Ca(NO <sub>3</sub> ) <sub>2</sub>                                   | 108.5              | 103.0 | 99.5  | 88.4 | 82.5 | 65.7 | 55.9 | 43.5 | 35.5 | 26.0 | 21.5 |
| ½Ca(OH) <sub>2</sub>                                                 |                    | 233   | 226   |      |      |      |      |      |      |      |      |
| ½CaSO <sub>4</sub>                                                   | 104.3              | 86.3  | 77.4  |      |      |      |      |      |      |      |      |
| ½CdBr <sub>2</sub>                                                   |                    | 86.5  | 76.3  | 53.2 | 44.6 | 25.3 | 18.3 | 12.5 | 9.1  | 6.8  | 5.3  |
| ½CdCl <sub>2</sub>                                                   |                    | 91    | 83    | 59   | 50   | 30.8 | 22.4 | 14.4 | 9.9  | 7.1  | 5.4  |
| ½CdI <sub>2</sub>                                                    |                    | 76.7  | 65.6  | 40.1 | 31.0 | 18.3 | 15.4 | 12.3 | 9.7  | 8.0  |      |
| ½Cd(NO <sub>3</sub> ) <sub>2</sub>                                   |                    | 100   | 96    | 86.4 | 80.8 | 63.9 | 54.5 | 41.0 | 31.4 | 23.7 | 17.6 |
| ½CdSO <sub>4</sub>                                                   | 97.7               | 79.7  | 70.3  | 49.6 | 42.2 | 28.7 | 23.6 | 17.7 | 14.0 | 11.0 | 8.35 |
| ⅓CeCl <sub>3</sub> (25°)                                             | 137.4              |       | 122.1 |      | 99.0 |      |      |      |      |      |      |
| ⅙Ce <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> (25°) | 85.5               | 54    | 45.8  | 29   |      |      |      |      |      |      |      |
| Chloroacetic acid (25°)                                              |                    |       |       |      | 42.9 | 20.2 | 13.6 | 8.1  | 5.6  | 4.2  | 3.3  |
| Citric acid                                                          | 88.4               | 54    | 42.5  | 22.0 | 16.1 | 7.3  | 5.4  |      |      |      |      |
| ½CoCl <sub>2</sub>                                                   |                    | 99.3  | 95.6  | 82.3 | 75.0 | 51.5 | 45.3 | 40.3 | 35.4 | 30.5 | 26.4 |
| ⅓CrCl <sub>3</sub>                                                   |                    |       |       |      |      | 68.6 | 56.8 | 44.8 | 35.2 |      |      |

**TABLE 8.35** Equivalent Conductivities of Electrolytes in Aqueous Solutions at 18°C (*Continued*)

| Electrolyte                                                | Concentration, <i>N</i> |       |       |       |       |       |       |      |       |      |       |
|------------------------------------------------------------|-------------------------|-------|-------|-------|-------|-------|-------|------|-------|------|-------|
|                                                            | 0.001                   | 0.005 | 0.01  | 0.05  | 0.1   | 0.5   | 1.0   | 2.0  | 3.0   | 4.0  | 5.0   |
| ½CrO <sub>3</sub> (H <sub>2</sub> CrO <sub>4</sub> ) (25°) | 201                     | 195   | 193   | 191   | 186   |       |       |      |       |      |       |
| CsCl                                                       | 130.7                   | 127.5 | 125.2 |       | 113.5 | 104.3 | 100.3 | 95.7 | 85.1  |      |       |
| ½Cu(OAc) <sub>2</sub> (25°)                                | 55.7                    | 50.6  | 47.2  | 34.9  | 28.4  |       |       |      |       |      |       |
| ½CuCl <sub>2</sub>                                         |                         |       |       |       |       |       |       | 41.2 | 31.5  | 24.5 | 19.1  |
| ½Cu(NO <sub>3</sub> ) <sub>2</sub> (15°)                   | 107.9                   | 97.1  | 93.7  | 83.7  | 78.2  | 67.5  | 56.8  | 45.4 | 35.3  | 27.8 | 21.4  |
| ½CuSO <sub>4</sub>                                         | 98.5                    | 81.0  | 71.7  | 53.6  | 43.8  | 30.5  | 25.6  | 19.7 | 16.5  |      |       |
| Dichloroacetic acid (25°)                                  |                         |       |       |       | 207.5 | 119   | 82    | 44.6 | 26.5  | 16.3 | 9.6   |
| ½FeCl <sub>2</sub> (25°)                                   | 131                     | 125   | 120   | 103   | 93    |       |       |      |       |      |       |
| ½FeCl <sub>3</sub>                                         |                         |       |       |       |       | 66.5  | 52.9  | 37.6 | 28.1  | 20.5 | 15.9  |
| ½FeSO <sub>4</sub>                                         | 82                      | 75    | 70    | 54    | 44.5  | 30.8  | 25.8  | 19.5 | 15.37 |      |       |
| Formic acid                                                | 125.6                   |       |       |       |       |       | 5.18  | 3.68 | 2.93  | 2.39 | 1.92  |
| H <sub>3</sub> AsO <sub>4</sub> (1 <i>M</i> ) (25°)        | 308.2                   | 230.0 | 187.0 | 103.4 | 80.4  |       |       |      |       |      |       |
| H <sub>3</sub> BO <sub>3</sub>                             | 13.5                    |       |       |       |       |       |       |      |       |      |       |
| HBr                                                        |                         |       |       |       | 356   | 306   | 282   | 243  | 214   | 179  |       |
| HBrO <sub>3</sub> (25°)                                    | 401                     | 387   | 373   | 272   | 156   |       |       |      |       |      |       |
| HCl                                                        | 377                     | 373   | 370   | 360   | 351   | 327   | 301   |      | 215   |      | 152.2 |
| HClO <sub>3</sub>                                          |                         |       |       |       | 343   | 317   | 292   | 247  | 207   |      |       |
| HClO <sub>4</sub> (25°)                                    | 413                     | 406   | 402   | 392   | 386   | 358   |       |      |       |      |       |
| HF                                                         |                         | 90    | 60    | 35.9  | 31.3  | 27.0  | 25.7  |      | 24.2  |      | 24.0  |
| HI                                                         |                         |       |       |       | 347   | 322   | 297   | 255  | 215   | 179  |       |
| HIO <sub>3</sub>                                           | 343.3                   | 332.8 | 323.9 |       | 253   | 175   | 141   | 106  | 87    | 71   |       |
| HNO <sub>3</sub>                                           | 375                     | 371   | 368   | 357   | 350   | 324   | 310   |      | 220   |      | 156   |
| H <sub>3</sub> PO <sub>4</sub> (1 <i>M</i> )               | 318                     | 279   | 255   |       |       |       | 66    |      | 53.1  |      | 51.3  |
| HSCN (25°)                                                 | 399                     | 394   | 390   | 377   | 370   |       |       |      |       |      |       |
| ½H <sub>2</sub> SO <sub>4</sub>                            | 361                     | 330   | 308   | 253   | 225   | 205   | 198   |      | 166.8 |      | 135.0 |
| ½HgCl <sub>2</sub>                                         |                         |       |       | 1.85  | 1.23  |       |       |      |       |      |       |
| ½InBr <sub>3</sub>                                         |                         |       |       |       | 53.9  | 37.0  | 28.7  | 19.8 | 14.4  | 10.1 |       |
| KOAc                                                       | 98.3                    | 95.7  | 94.0  | 87.7  | 83.8  | 71.6  | 63.4  | 50.0 | 40.7  | 31.4 | 24.5  |
| KBr                                                        | 129.4                   | 126.4 | 124.4 | 117.8 | 114.2 | 105.4 | 102.5 | 98.0 | 93.3  | 87.9 |       |
| KBrO <sub>3</sub>                                          | 109.9                   | 106.9 | 104.7 | 97.3  | 93.0  |       |       |      |       |      |       |
| ½K <sub>3</sub> citrate                                    |                         | 109.9 | 103   | 87.8  | 80.8  |       |       |      |       |      |       |

|                                                  |       |       |       |       |       |                    |                    |       |       |      |       |
|--------------------------------------------------|-------|-------|-------|-------|-------|--------------------|--------------------|-------|-------|------|-------|
| KCl                                              | 127.3 | 124.4 | 122.4 | 115.8 | 112.0 | 102.4              | 98.3               | 92.0  | 88.9  |      |       |
| KClO <sub>3</sub>                                | 116.9 | 113.6 | 111.6 | 103.7 | 99.2  | 85.3               |                    |       |       |      |       |
| KClO <sub>4</sub> (25°)                          | 137.9 | 134.2 | 131.5 | 121.6 | 115.2 |                    |                    |       |       |      |       |
| KCN (15°)                                        |       |       |       |       |       | 104.2              | 99.7               |       |       |      |       |
| ½K <sub>2</sub> CO <sub>3</sub>                  | 133.0 | 121.6 | 115.5 | 100.7 | 94.1  | 77.8               | 70.7               | 65.0  | 55.6  | 49.2 | 42.9  |
| ½K <sub>2</sub> C <sub>2</sub> O <sub>4</sub>    | 122.4 | 116.7 | 112.5 | 100.8 | 94.9  | 80.4               | 73.7               |       |       |      |       |
| ½K <sub>2</sub> CrO <sub>4</sub>                 |       |       |       |       | 100.5 | 86.4               | 79.5               | 72.0  | 59.9  |      |       |
| ½K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>   |       |       |       |       | 98.2  | 85.4               |                    |       |       |      |       |
| KF                                               | 108.9 | 106.2 | 104.3 | 97.7  | 94.0  | 82.6               | 76.0               | 63.4  | 56.5  | 51.7 | 46.5  |
| ⅓K <sub>3</sub> [Fe(CN) <sub>6</sub> ]           | 163.1 | 150.7 |       |       |       |                    |                    |       |       |      |       |
| ¼K <sub>4</sub> [Fe(CN) <sub>6</sub> ]           | 167.2 | 146.1 | 134.8 | 107.7 | 97.9  |                    |                    |       |       |      |       |
| KHCO <sub>3</sub> (25°)                          | 115.3 | 112.2 | 110.1 |       |       | 86.5               | 78.9               |       |       |      |       |
| KH phthalate                                     | 119.3 | 103.7 | 99.9  | 89.3  | 83.8  |                    |                    |       |       |      |       |
| KHS                                              |       |       |       |       |       | 92.5               | 91.7               | 86.4  | 80.7  |      | 69.3  |
| KHSO <sub>4</sub>                                |       |       |       |       |       | 21.0               | 18.4               | 15.2  |       |      |       |
| KH <sub>2</sub> PO <sub>4</sub> (1 M) (25°)      | 107.1 | 100.8 | 98.0  | 90.7  | 85.6  | 60.0 <sup>18</sup> | 45.8 <sup>18</sup> |       |       |      |       |
| KI                                               | 128.2 | 125.3 | 123.4 | 117.3 | 114.0 | 106.2              | 103.6              | 101.3 | 96.4  | 89.0 | 81.2  |
| KIO <sub>3</sub>                                 | 96.0  | 93.2  | 91.2  | 84.1  | 79.7  |                    |                    |       |       |      |       |
| KIO <sub>4</sub> (25°)                           | 124.9 | 121.2 | 118.5 | 106.7 | 98.1  |                    |                    |       |       |      |       |
| KMnO <sub>4</sub> (25°)                          | 133.3 |       | 126.5 |       | 113   |                    |                    |       |       |      |       |
| KNO <sub>3</sub>                                 | 123.6 | 120.5 | 118.2 | 109.9 | 104.8 | 89.2               | 80.5               | 69.4  | 61.3  |      |       |
| KOH                                              | 234   | 230   | 228   | 219   | 213   | 197                | 184                |       | 140.6 |      | 105.8 |
| KReO <sub>4</sub> (25°)                          | 125.1 | 121.3 | 118.5 | 106.4 | 97.4  |                    |                    |       |       |      |       |
| ½K <sub>2</sub> S                                |       |       |       |       |       |                    | 135.6              | 119.7 | 108.3 | 97.2 | 86.1  |
| KSCN                                             | 118.6 | 115.8 | 113.9 | 107.7 | 104.3 | 95.7               | 91.6               | 86.8  | 74.6  |      |       |
| ½K <sub>2</sub> SO <sub>4</sub>                  | 126.9 | 120.3 | 115.8 | 101.9 | 94.9  | 78.5               | 71.6               |       |       |      |       |
| ½LaCl <sub>3</sub> (25°)                         | 137.0 | 127.5 | 121.8 | 106.2 | 99.1  |                    |                    |       |       |      |       |
| ⅓La(NO <sub>3</sub> ) <sub>3</sub>               |       |       |       | 86.1  | 72.1  | 65.4               | 54.0               | 39.1  | 28.5  | 19.9 |       |
| ⅙La <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> |       |       |       | 25.7  | 21.5  |                    |                    |       |       |      |       |
| Lactic acid                                      | 108.9 | 53.5  | 39    | 18.1  | 13.2  |                    |                    |       |       |      |       |
| LiOAc                                            |       |       |       |       | 51.3  | 37.7               | 28.9               | 18.2  | 11.9  | 7.2  |       |
| LiBr                                             |       |       |       | 87.9  | 84.4  | 73.9               | 67.2               | 57.7  |       | 44.2 |       |
| LiCl                                             | 96.5  | 93.9  | 92.1  | 86.1  | 82.4  | 70.7               | 63.4               | 53.1  | 45.3  |      | 33.3  |
| LiClO <sub>4</sub> (25°)                         | 103.4 | 100.6 | 98.6  | 92.2  | 88.6  |                    |                    |       |       |      |       |
| ½Li <sub>2</sub> CO <sub>3</sub>                 |       |       |       | 64.2  | 59.1  |                    |                    |       |       |      |       |
| LiI                                              |       |       |       |       |       | 75.3               | 69.2               | 61.0  |       |      |       |
| LiIO <sub>3</sub>                                | 65.3  | 62.9  | 61.2  | 55.3  | 51.5  | 39.0               | 31.2               | 21.4  | 14.6  |      |       |

**TABLE 8.35** Equivalent Conductivities of Electrolytes in Aqueous Solutions at 18°C (*Continued*)

| Electrolyte                                                   | Concentration, <i>N</i> |                     |                     |                     |                    |       |       |       |      |      |      |
|---------------------------------------------------------------|-------------------------|---------------------|---------------------|---------------------|--------------------|-------|-------|-------|------|------|------|
|                                                               | 0.001                   | 0.005               | 0.01                | 0.05                | 0.1                | 0.5   | 1.0   | 2.0   | 3.0  | 4.0  | 5.0  |
| LiNO <sub>3</sub>                                             | 92.9                    | 90.3                | 88.6                | 82.7                | 79.2               | 68.0  | 60.8  | 50.3  | 34.9 | 27.3 |      |
| LiOH                                                          |                         |                     |                     |                     |                    | 149.0 | 134.5 | 113.5 | 95.7 |      |      |
| ½Li <sub>2</sub> SO <sub>4</sub>                              | 96.4                    |                     | 86.9                | 74.7                | 68.2               | 50.5  | 41.3  | 30.7  | 23.3 | 18.1 | 13.9 |
| ½MgCl <sub>2</sub>                                            | 106.4                   | 101.3               | 98.1                | 88.5                | 83.4               | 69.6  | 61.5  | 52.3  | 43.3 | 35.0 | 28.0 |
| ½Mg(NO <sub>3</sub> ) <sub>2</sub>                            | 102.6                   | 97.7                | 94.7                | 85.3                | 80.5               | 67.0  | 59.0  | 47.0  | 39.8 |      |      |
| ½MgSO <sub>4</sub>                                            | 99.8                    | 84.5                | 76.2                | 56.9                | 49.7               | 35.4  | 28.9  | 23.0  | 17.3 | 12.9 | 9.3  |
| ½MnCl <sub>2</sub>                                            |                         |                     |                     |                     | 86.0               | 68.5  | 61.0  | 48.5  | 38.8 | 30.2 | 23.0 |
| ½MnSO <sub>4</sub>                                            |                         |                     |                     |                     |                    | 27.6  | 24.4  | 18.3  | 14.0 | 10.5 | 7.3  |
| NH <sub>3</sub> (aq)                                          | 28.0                    | 13.2                | 9.6                 | 4.6                 | 3.3                | 1.35  | 0.89  |       | 0.36 |      | 0.20 |
| NH <sub>4</sub> OAc                                           |                         | 92.9                | 91.4                | 84.9                |                    | 60.5  | 54.7  | 42.9  | 34.0 | 26.5 |      |
| NH <sub>4</sub> Cl                                            | 127.3                   | 124.3               | 122.1               | 115.2               | 110.7              | 101.4 | 97.0  | 92.1  | 88.2 | 85.0 | 80.7 |
| NH <sub>4</sub> F                                             |                         |                     |                     |                     | 90.1               | 74.5  | 65.7  | 55.3  | 47.9 | 42.2 |      |
| NH <sub>4</sub> I                                             |                         |                     |                     | 118.0               | 115.0              | 106.0 | 103.1 | 100.0 |      | 91.4 | 84.5 |
| NH <sub>4</sub> NO <sub>3</sub>                               | 124.5                   |                     | 118.0               | 110.0               | 106.6              | 94.5  | 88.8  | 85.1  |      | 71.9 | 47.6 |
| NH <sub>4</sub> SCN                                           |                         |                     |                     |                     | 104.3              | 94.0  | 89.9  | 84.7  | 79.2 | 74.0 |      |
| ½(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>              |                         | 120.0               | 116.5               |                     | 89.0               | 79.5  | 73.0  | 65.0  |      | 55.2 |      |
| NaOAc                                                         | 75.2                    | 72.4                | 70.2                | 64.2                | 61.1               | 49.4  | 41.2  | 29.8  | 21.5 | 15.3 | 10.5 |
| NaBr                                                          |                         |                     |                     | 99.1                | 96.0               | 84.6  | 78.1  | 69.1  |      | 53.0 |      |
| NaBrO <sub>3</sub>                                            |                         |                     |                     |                     |                    | 61.8  | 54.5  | 44.1  |      |      |      |
| Na <i>n</i> -butyrate (25°)                                   | 80.3                    | 77.6                | 75.8                | 69.3                | 65.3               |       |       |       |      |      |      |
| NaCl                                                          | 106.5                   | 103.8               | 102.0               | 95.7                | 92.0               | 80.9  | 74.3  | 64.8  | 56.5 | 49.4 | 42.7 |
| NaClO <sub>4</sub>                                            | 114.9 <sup>25</sup>     | 111.7 <sup>25</sup> | 109.6 <sup>25</sup> | 102.4 <sup>25</sup> | 98.4 <sup>25</sup> | 71.7  | 65.0  | 55.1  | 46.0 | 38.8 |      |
| ½Na <sub>2</sub> CO <sub>3</sub>                              | 112                     | 102.5               | 96.2                | 80.3                | 72.9               | 54.5  | 45.5  | 34.5  | 27.2 |      |      |
| ½Na <sub>2</sub> CrO <sub>4</sub>                             |                         |                     |                     |                     | 82.5               | 66.4  | 57.7  | 46.6  | 38.3 | 31.1 |      |
| ½Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> (25°)         |                         | 103                 |                     | 98.3                | 94.9               |       |       |       |      |      |      |
| NaF                                                           | 87.8                    | 85.2                | 83.5                | 77.0                | 73.1               | 60.0  | 51.9  |       |      |      |      |
| ¼Na <sub>4</sub> [Fe(CN) <sub>6</sub> ] (25°)                 |                         | 129.6               | 120.0               | 97.0                | 88.2               |       |       |       |      |      |      |
| Na formate                                                    | 88.6                    |                     |                     |                     |                    | 61.4  | 53.7  | 43.1  | 34.8 | 28.2 |      |
| NaHCO <sub>3</sub> (25°)                                      | 93.5                    | 90.5                | 88.4                | 80.6                | 76.0               |       |       |       |      |      |      |
| ⅓Na <sub>2</sub> HPO <sub>4</sub>                             | 58.4                    |                     | 54.0                |                     | 44.0               | 33.5  | 28.0  |       |      |      |      |
| NaH <sub>2</sub> PO <sub>4</sub>                              | 67.9                    | 65.8                | 64.4                | 57.8                | 54.1               |       |       |       |      |      |      |
| ¼Na <sub>2</sub> H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> | 41.1                    | 39.4                | 38.2                | 34.6                | 32.5               | 25.4  |       |       |      |      |      |
| NaI                                                           | 124.2                   | 121.2               | 119.2               | 112.8               | 108.8              | 97.5  | 89.9  | 78.6  | 69.9 | 62.2 |      |

|                                        |       |       |       |       |       |       |       |       |       |      |      |
|----------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|
| NaIO <sub>3</sub>                      | 75.2  | 72.6  | 70.9  | 64.4  | 60.5  |       |       |       |       |      |      |
| ½Na <sub>2</sub> MoO <sub>4</sub>      | 120.8 | 113   | 110   |       |       |       |       |       |       |      |      |
| NaN <sub>3</sub> (25°)                 | 117.1 | 113.8 | 110.5 | 101.3 | 95.7  |       | 68.0  |       |       |      |      |
| NaNO <sub>2</sub> (25°)                |       |       |       |       |       |       | 75.9  | 63.1  | 53.6  |      | 39.7 |
| NaNO <sub>3</sub>                      | 102.9 | 100.1 | 98.2  | 91.4  | 87.2  | 74.1  | 65.9  | 54.5  | 46.0  | 39.0 |      |
| NaOH                                   | 208   | 203   | 200   | 190   | 183   | 172   | 160   |       | 108.0 |      | 69.0 |
| Na picrate (25°)                       | 78.6  | 75.7  | 73.7  | 66.3  | 61.8  |       |       |       |       |      |      |
| ⅓Na <sub>3</sub> PO <sub>4</sub>       | 125   | 122   | 119   | 91    |       |       |       |       |       |      |      |
| Na propionate (25°)                    | 83.5  | 80.9  | 79.1  |       |       |       |       |       |       |      |      |
| ½Na <sub>2</sub> S                     |       |       |       |       |       | 117.0 | 104.3 | 85.0  | 71.0  | 59.0 | 47.2 |
| NaSCN                                  |       |       |       |       |       | 74.3  | 68.9  | 59.8  | 50.9  | 43.7 |      |
| ½Na <sub>2</sub> SiO <sub>3</sub>      | 144   | 139   | 136   | 124   | 116   | 88    | 72    | 51    | 38    | 27   | 19   |
| ½Na <sub>2</sub> SO <sub>4</sub>       | 106.7 | 100.8 | 96.8  | 83.9  | 78.4  | 59.7  | 50.8  | 40.0  | 33.5  |      |      |
| (mono) Na tartrate                     | 120   | 81.5  | 74.8  | 64.3  | 60.4  |       |       |       |       |      |      |
| ½Na <sub>2</sub> WO <sub>4</sub> (25°) | 116.1 | 109.2 | 104.8 | 92.2  | 85.8  |       |       |       |       |      |      |
| ½NiSO <sub>4</sub>                     | 96.3  | 79.5  | 70.8  | 51.0  | 43.8  | 30.4  | 25.1  | 19.3  | 15.1  |      |      |
| ½Oxalic acid                           | 180.7 |       | 158.2 | 132.9 | 116.9 | 75.9  | 59.4  |       |       |      |      |
| ½Pb(NO <sub>3</sub> ) <sub>2</sub>     | 116.1 | 108.6 | 103.5 | 86.3  | 77.3  | 53.2  | 42.0  | 31.0  |       |      |      |
| Propionic acid                         |       |       |       |       |       | 1.57  | 1.00  | 0.54  |       | 0.20 |      |
| RbCl                                   | 130.3 | 127.4 | 125.3 | 117.8 | 113.9 |       | 101.9 | 97.1  | 92.7  | 87.2 |      |
| RbOH                                   |       |       |       |       | 220.6 |       | 192.0 | 170.0 | 148.3 |      |      |
| ¼SnCl <sub>4</sub>                     |       |       |       |       |       | 216.8 | 121.7 | 66.9  | 47.9  | 32.7 |      |
| ½SrCl <sub>2</sub>                     | 114.5 | 108.9 | 105.4 | 94.4  | 90.2  | 75.7  | 68.5  | 58.7  | 49.9  | 42.2 |      |
| ½Sr(NO <sub>3</sub> ) <sub>2</sub>     | 108.3 | 102.7 | 99.0  | 87.3  | 80.9  | 62.7  | 52.1  | 38.0  | 29.3  | 29.3 | 16.4 |
| Tartaric acid (15°)                    |       |       |       |       |       |       | 7.03  | 4.58  | 3.32  | 2.48 | 1.83 |
| ¼ThCl <sub>4</sub>                     |       |       |       |       |       | 61.0  | 54.0  | 44.3  | 36.3  | 29.8 |      |
| TiCl                                   | 128.2 | 123.7 | 120.2 |       |       |       |       |       |       |      |      |
| TiF                                    | 113.3 | 108.2 | 105.4 | 97.4  | 92.6  | 78.8  | 71.5  | 62.7  |       |      |      |
| TiNO <sub>3</sub>                      | 124.7 | 121.1 | 118.4 | 107.9 | 101.2 |       |       |       |       |      |      |
| ½Ti <sub>2</sub> SO <sub>4</sub>       | 127.4 | 118.4 | 112.3 | 92.7  | 83.1  |       |       |       |       |      |      |
| Trichloroacetic acid (25°)             |       |       |       |       |       | 273   | 207   | 127   | 79    | 44   | 19   |
| ½UO <sub>2</sub> F <sub>2</sub> (25°)  | 26.10 | 12.31 | 9.17  | 5.43  | 4.74  | 3.75  | 3.22  |       |       |      |      |
| ½UO <sub>2</sub> SO <sub>4</sub> (25°) | 106.5 | 63.2  | 49.2  | 27.6  | 22.2  | 14.4  | 11.6  |       |       |      | 2.7  |
| ⅓YCl <sub>3</sub> (25°)                | 129   | 122   | 118   | 109   |       |       |       |       |       |      |      |
| ½Zn(OAc) <sub>2</sub> (25°)            | 83    | 77    | 73    | 58    | 49    |       |       |       |       |      |      |
| ½ZnCl <sub>2</sub>                     | 107   | 101   | 98    | 87    | 82    | 65    | 55    | 39.6  | 29.6  | 23.2 | 18.5 |
| ½Zn(NO <sub>3</sub> ) <sub>2</sub>     | 120   | 114   | 111   | 100   |       |       |       |       |       |      |      |
| ½ZnSO <sub>4</sub>                     | 98.4  | 82.1  | 73.2  | 53.0  | 45.6  | 32.3  | 26.6  | 20.0  | 15.9  | 12.0 | 9.0  |



**TABLE 8.36** Conductivity of Very Pure Water at Various Temperatures and the Equivalent Conductances of Hydrogen and Hydroxyl Ions

| Temp., °C | Conductivity, $\mu\text{S} \cdot \text{cm}^{-1}$ | Resistivity, $\text{M}\Omega \cdot \text{cm}$ | Equivalent conductance,<br>$\text{cm}^2 \cdot \text{ohm}^{-1} \cdot \text{equivalent}^{-1}$ |                          |
|-----------|--------------------------------------------------|-----------------------------------------------|---------------------------------------------------------------------------------------------|--------------------------|
|           |                                                  |                                               | $\lambda^0, \text{H}^+$                                                                     | $\lambda^0, \text{OH}^-$ |
| 0         | 0.011 61                                         | 86.14                                         | 224.1                                                                                       | 117.8                    |
| 5         | 0.016 61                                         | 60.21                                         | 250.0                                                                                       | 133.6                    |
| 10        | 0.023 15                                         | 43.21                                         | 275.6                                                                                       | 149.6                    |
| 15        | 0.031 53                                         | 31.71                                         | 300.9                                                                                       | 165.9                    |
| 18        | 0.037 54                                         | 26.64                                         | 315.8                                                                                       | 491.6                    |
| 20        | 0.042 05                                         | 23.78                                         | 325.7                                                                                       | 182.5                    |
| 25        | 0.055 08                                         | 18.15                                         | 350.1                                                                                       | 199.2                    |
| 30        | 0.070 96                                         | 14.09                                         | 374.0                                                                                       | 216.1                    |
| 35        | 0.090 05                                         | 11.10                                         | 397.4                                                                                       | 233.0                    |
| 40        | 0.112 7                                          | 8.88                                          | 420.0                                                                                       | 267.2                    |
| 45        | 0.139 3                                          | 7.18                                          | 442.0                                                                                       | 267.2                    |
| 50        | 0.170 2                                          | 5.88                                          | 463.3                                                                                       | 284.3                    |
| 55        | 0.205 5                                          | 4.86                                          | 483.8                                                                                       | 301.4                    |
| 60        | 0.245 7                                          | 4.06                                          | 503.4                                                                                       | 318.5                    |
| 65        | 0.291 2                                          | 3.43                                          | 522.0                                                                                       | 335.4                    |
| 70        | 0.341 6                                          | 2.93                                          | 539.7                                                                                       | 352.2                    |
| 75        | 0.397 8                                          | 2.51                                          | 556.4                                                                                       | 368.8                    |
| 80        | 0.459 3                                          | 2.18                                          | 572.0                                                                                       | 385.2                    |
| 85        | 0.525 8                                          | 1.90                                          | 586.4                                                                                       | 401.4                    |
| 90        | 0.597 7                                          | 1.67                                          | 599.6                                                                                       | 417.3                    |
| 95        | 0.675 3                                          | 1.48                                          | 611.6                                                                                       | 432.8                    |
| 100       | 0.756 9                                          | 1.32                                          | 622.2                                                                                       | 448.1                    |
| 150       | 1.84                                             | 0.543                                         |                                                                                             |                          |
| 200       | 2.99                                             | 0.334                                         | 824                                                                                         | 701                      |
| 250       | 3.31                                             | 0.302                                         |                                                                                             |                          |
| 300       | 2.42                                             | 0.413                                         | 894                                                                                         | 821                      |

**Source:** Data from T. S. Light and S. L. Licht, *Anal. Chem.*, 59:2327–2330 (1987).

8.7.1 Common Conductance Relations\*

*Conductivity.* The standard unit of conductance is electrolytic conductivity (formerly called specific conductance)  $\kappa$ , which is defined as the reciprocal of the resistance [ $\Omega^{-1}$ ] of a 1-m cube of liquid at a specified temperature [ $\Omega^{-1} \cdot \text{m}^{-1}$ ]. See Table 8.33 and the definition of the cell constant.

In accurate work at low concentrations it is necessary to subtract the conductivity of the pure solvent (Table 8.34) from that of the solution to obtain the conductivity due to the electrolyte.

*Resistivity (Specific Resistance)*

$$\rho = \frac{1}{\kappa} \quad [\Omega \cdot \text{m}]$$

\* SI units are in brackets.

*Conductance of an Electrolyte Solution*

$$\frac{1}{R} = \kappa \frac{S}{d} \quad [\Omega^{-1}]$$

where  $S$  is the surface area of the electrode, or the mean cross-sectional area of the solution [ $\text{m}^2$ ], and  $d$  is the mean distance between the electrodes [ $\text{m}$ ].

*Equivalent Conductivity*

$$\Lambda = \frac{\kappa}{C} \quad [\Omega^{-1} \cdot \text{m}^2 \cdot \text{equiv}^{-1}]$$

In the older literature,  $C$  is the concentration in equivalents per liter. The volume of the solution in cubic centimeters per equivalent is equal to  $1000/C$ , and  $\Lambda = 1000 \kappa/C$ , the units employed in Table 8.32 [ $\Omega^{-1} \cdot \text{cm}^2 \cdot \text{equiv}^{-1}$ ]. The formula unit used in expressing the concentration must be specified; for example,  $\text{NaCl}$ ,  $\frac{1}{2}\text{K}_2\text{SO}_4$ ,  $\frac{1}{3}\text{LaCl}_3$ .

The equivalent conductivity of an electrolyte is the sum of contributions of the individual ions. At infinite dilution:  $\Lambda^\circ = \lambda_c^\circ + \lambda_a^\circ$ , where  $\lambda_c^\circ$  and  $\lambda_a^\circ$  are the ionic conductances of cations and anions, respectively, at infinite dilution (Table 8.35).

*Ionic Mobility and Ionic Equivalent Conductivity*

$$\lambda_c = Fu_c \quad \text{and} \quad \lambda_a = Fu_a \quad [\Omega^{-1} \cdot \text{m}^2 \cdot \text{equiv}^{-1}]$$

where  $F$  is the Faraday constant, and  $u_c$ ,  $u_a$  are the ionic mobilities [ $\text{m}^2 \cdot \text{s}^{-1} \cdot \text{V}^{-1}$ ].

$$\Lambda = \alpha F(u_c + u_a) = \alpha(\lambda_c + \lambda_a)$$

where  $\alpha$  is the degree of electrolytic dissociation,  $\Lambda/\Lambda^\circ$ . The electric mobility  $u$  of a species is the magnitude of the velocity in an electric field [ $\text{m} \cdot \text{s}^{-1}$ ] divided by the magnitude of the strength of the electric field  $E$  [ $\text{V} \cdot \text{m}^{-1}$ ].

*Ostwald Dilution Law*

$$K_d = \frac{\alpha^2 C}{1 - \alpha}$$

where  $K_d$  is the dissociation constant of the weak electrolyte. In general for an electrolyte which yields  $n$  ions:

$$K_d = \frac{C^{(n-1)}\Lambda^n}{\Lambda^\circ(n-1)(\Lambda^\circ - \Lambda)}$$

*Transference Numbers or Hittorf Transport Numbers*

$$T_c = \frac{\lambda_c}{\lambda_c + \lambda_a} \quad T_a = \frac{\lambda_a}{\lambda_c + \lambda_a} \quad T_c + T_a = 1$$

$$\frac{T_c}{T_a} = \frac{u_c}{u_a} = \frac{\lambda_c}{\lambda_a}$$

$$\lambda_c = T_c \Lambda \quad \lambda_a = T_a \Lambda$$

---

# SECTION 9

---

## PHYSICOCHEMICAL RELATIONSHIPS

---

|                  |                                                               |            |
|------------------|---------------------------------------------------------------|------------|
| <b>9.1</b>       | <b>LINEAR FREE ENERGY RELATIONSHIPS</b>                       | <b>9.2</b> |
| <b>Table 9.1</b> | <b>Hammett and Taft Substituent Constants</b>                 | <b>9.2</b> |
| <b>Table 9.2</b> | <b><math>pK'_s</math> and Rho Values for Hammett Equation</b> | <b>9.6</b> |
| <b>Table 9.3</b> | <b><math>pK'_s</math> and Rho Values for Taft Equation</b>    | <b>9.7</b> |
| <b>Table 9.4</b> | <b>Special Hammett Sigma Constants</b>                        | <b>9.8</b> |

## 9.1 LINEAR FREE ENERGY RELATIONSHIPS

Many equilibrium and rate processes can be systematized when the influence of each substituent on the reactivity of substrates is assigned a characteristic constant  $\sigma$  and the reaction parameter  $\rho$  is known or can be calculated. The Hammett equation

$$\log \frac{K}{K^\circ} = \sigma \rho$$

describes the behavior of many *meta*- and *para*-substituted aromatic species. In this equation  $K^\circ$  is the acid dissociation constant of the reference in aqueous solution at 25°C and  $K$  is the corresponding constant for the substituted acid. Separate sigma values are defined by this reaction for *meta* and *para* substituents and provide a measure of the total electronic influence (polar, inductive, and resonance effects) in the absence of conjugation effects. Sigma constants are not valid of substituents *ortho* to the reaction center because of anomalous (mainly steric) effects. The inductive effect is transmitted about equally to the *meta* and *para* positions. Consequently,  $\sigma_m$  is an approximate measure of the size of the inductive effect of a given substituent and  $\sigma_p - \sigma_m$  is an approximate measure of a substituent's resonance effect. Values of Hammett sigma constants are listed in Table 9.1.

Taft sigma values  $\sigma^*$  perform a similar function with respect to aliphatic and alicyclic systems. Values of  $\sigma^*$  are listed in Table 9.1.

The reaction parameter  $\rho$  depends upon the reaction series but not upon the substituents employed. Values of the reaction parameter for some aromatic and aliphatic systems are given in Tables 9.2 and 9.3.

Since substituent effects in aliphatic systems and in *meta* positions in aromatic systems are essentially inductive in character,  $\sigma^*$  and  $\sigma_m$  values are often related by the expression  $\sigma_m = 0.217\sigma^* - 0.106$ . Substituent effects fall off with increasing distance from the reaction center; generally a factor of 0.36 corresponds to the interposition of a  $-\text{CH}_2-$  group, which enables  $\sigma^*$  values to be estimated for  $\text{R}-\text{CH}_2-$  groups not otherwise available.

**TABLE 9.1** Hammett and Taft Substituent Constants

| Substituent                                                | Hammett constants |            | Taft constant $\sigma^*$ |
|------------------------------------------------------------|-------------------|------------|--------------------------|
|                                                            | $\sigma_m$        | $\sigma_p$ |                          |
| $-\text{AsO}_3\text{H}^-$                                  | -0.09             | -0.02      | 0.06                     |
| $-\text{B}(\text{OH})_2$                                   | 0.01              | 0.45       |                          |
| $-\text{Br}$                                               | 0.39              | 0.23       | 2.84                     |
| $-\text{CH}_2\text{Br}$                                    |                   |            | 1.00                     |
| <i>m</i> - $\text{BrC}_6\text{H}_4-$                       |                   | 0.09       |                          |
| <i>p</i> - $\text{BrC}_6\text{H}_4-$                       |                   | 0.08       |                          |
| $-\text{CH}_3$                                             | -0.07             | -0.17      | 0.0                      |
| $-\text{CH}_2\text{CH}_3$                                  | -0.07             | -0.15      | -0.10                    |
| $-\text{CH}_2\text{CH}_2\text{CH}_3$                       | -0.05             | -0.15      | -0.12                    |
| $-\text{CH}(\text{CH}_3)_2$                                | -0.07             | -0.15      | -0.19                    |
| $-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$            | -0.07             | -0.16      | -0.13                    |
| $-\text{CH}_2\text{CH}(\text{CH}_3)_2$                     | -0.07             | -0.12      | -0.13                    |
| $-\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$            |                   | -0.12      | -0.19                    |
| $-\text{C}(\text{CH}_3)_3$                                 | -0.10             | -0.20      | -0.30                    |
| $-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ |                   |            | -0.25                    |
| $-\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$          |                   |            | -0.17                    |

**TABLE 9.1** Hammett and Taft Substituent Constants (*Continued*)

| Substituent                                                                                      | Hammett constants |            | Taft constant<br>$\sigma^*$ |
|--------------------------------------------------------------------------------------------------|-------------------|------------|-----------------------------|
|                                                                                                  | $\sigma_m$        | $\sigma_p$ |                             |
| —CH <sub>2</sub> C(CH <sub>3</sub> ) <sub>3</sub>                                                |                   | −0.23      | −0.12                       |
| —CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> |                   |            | −0.37                       |
| Cyclopropyl—                                                                                     | −0.07             | −0.21      |                             |
| Cyclohexyl—                                                                                      |                   |            | −0.15                       |
| —3,4-(CH <sub>2</sub> ) <sub>2</sub> (fused)                                                     |                   | −0.26      |                             |
| —3,4-(CH <sub>2</sub> ) <sub>3</sub> — (fused ring)                                              |                   | −0.48      |                             |
| —3,4-(CH) <sub>4</sub> — (fused ring)                                                            | 0.06              | 0.04       |                             |
| —CH=CH <sub>2</sub>                                                                              | 0.02              |            | 0.56                        |
| —CH=C(CH <sub>3</sub> ) <sub>2</sub>                                                             |                   |            | 0.19                        |
| —CH=CHCH <sub>3</sub> , <i>trans</i>                                                             |                   |            | 0.36                        |
| —CH <sub>2</sub> —CH=CH <sub>2</sub>                                                             |                   |            | 0.0                         |
| —CH=CHC <sub>6</sub> H <sub>5</sub>                                                              | 0.14              | −0.05      | 0.41                        |
| —C≡CH                                                                                            | 0.21              | 0.23       | 2.18                        |
| —C≡CC <sub>6</sub> H <sub>5</sub>                                                                | 0.14              | 0.16       | 1.35                        |
| —CH <sub>2</sub> —C≡CH                                                                           |                   |            | 0.81                        |
| —C <sub>6</sub> H <sub>5</sub>                                                                   | 0.06              | −0.01      | 0.60                        |
| <i>p</i> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> —                                        |                   | −0.5       |                             |
| Naphthyl— (both 1- and 2-)                                                                       |                   |            | 0.75                        |
| —CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>                                                   |                   | 0.46       | 0.22                        |
| —CH <sub>2</sub> CH <sub>2</sub> —C <sub>6</sub> H <sub>5</sub>                                  |                   |            | −0.06                       |
| —CH(CH <sub>3</sub> )C <sub>6</sub> H <sub>5</sub>                                               |                   |            | 0.37                        |
| —CH(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>                                                 |                   |            | 0.41                        |
| —CH <sub>2</sub> —C <sub>10</sub> H <sub>7</sub>                                                 |                   |            | 0.44                        |
| 2-Furoyl—                                                                                        |                   |            | 0.25                        |
| 3-Indolyl—                                                                                       |                   |            | −0.06                       |
| 2-Thienyl—                                                                                       |                   |            | 1.31                        |
| 2-Thienylmethylene—                                                                              |                   |            | 0.31                        |
| —CHO                                                                                             | 0.36              | 0.22       |                             |
| —COCH <sub>3</sub>                                                                               | 0.38              | 0.50       | 1.65                        |
| —COCH <sub>2</sub> CH <sub>2</sub>                                                               |                   | 0.48       |                             |
| —COCH(CH <sub>3</sub> ) <sub>2</sub>                                                             |                   | 0.47       |                             |
| —COC(CH <sub>3</sub> ) <sub>3</sub>                                                              |                   | 0.32       |                             |
| —COCF <sub>3</sub>                                                                               | 0.65              |            | 3.7                         |
| —COC <sub>6</sub> H <sub>5</sub>                                                                 | 0.34              | 0.46       | 2.2                         |
| —CONH <sub>2</sub>                                                                               | 0.28              | 0.36       | 1.68                        |
| —CONHC <sub>6</sub> H <sub>5</sub>                                                               |                   |            | 1.56                        |
| —CH <sub>2</sub> COCH <sub>3</sub>                                                               |                   |            | 0.60                        |
| —CH <sub>2</sub> CONH <sub>2</sub>                                                               |                   |            | 0.31                        |
| —CH <sub>2</sub> CH <sub>2</sub> CONH <sub>2</sub>                                               |                   |            | 0.19                        |
| —CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CONH <sub>2</sub>                               |                   |            | 0.12                        |
| —CH <sub>2</sub> CONHC <sub>6</sub> H <sub>5</sub>                                               |                   |            | 0.0                         |
| —COO <sup>−</sup>                                                                                | −0.1              | 0.0        | −1.06                       |
| —COOH                                                                                            | 0.36              | 0.43       | 2.08                        |
| —CO—OCH <sub>3</sub>                                                                             | 0.32              | 0.39       | 2.00                        |
| —CO—OCH <sub>2</sub> CH <sub>3</sub>                                                             | 0.37              | 0.45       | 2.12                        |
| —CH <sub>2</sub> CO—OCH <sub>3</sub>                                                             |                   |            | 1.06                        |
| —CH <sub>2</sub> CO—OCH <sub>2</sub> CH <sub>3</sub>                                             |                   |            | 0.82                        |
| —CH <sub>2</sub> COO                                                                             |                   |            | −0.06                       |
| —CH <sub>2</sub> CH <sub>2</sub> COOH                                                            | −0.03             | −0.07      |                             |
| —Cl                                                                                              | 0.37              | 0.23       | 2.96                        |
| —CCl <sub>3</sub>                                                                                | 0.47              |            | 2.65                        |
| —CHCl <sub>2</sub>                                                                               |                   |            | 1.94                        |

**TABLE 9.1** Hammett and Taft Substituent Constants (*Continued*)

| Substituent                                                      | Hammett constants |            | Taft constant<br>$\sigma^*$ |
|------------------------------------------------------------------|-------------------|------------|-----------------------------|
|                                                                  | $\sigma_m$        | $\sigma_p$ |                             |
| —CH <sub>2</sub> Cl                                              | 0.12              | 0.18       | 1.05                        |
| —CH <sub>2</sub> CH <sub>2</sub> Cl                              |                   |            | 0.38                        |
| —CH <sub>2</sub> CCl <sub>3</sub>                                |                   |            | 0.75                        |
| —CH <sub>2</sub> CH <sub>2</sub> CCl <sub>3</sub>                |                   |            | 0.25                        |
| —CH=CCl <sub>2</sub>                                             |                   |            | 1.00                        |
| —CH <sub>2</sub> CH=CCl <sub>2</sub>                             |                   |            | 0.19                        |
| <i>p</i> -ClC <sub>6</sub> H <sub>4</sub> —                      |                   | 0.08       |                             |
| —F                                                               | 0.34              | 0.06       | 3.21                        |
| —CF <sub>3</sub>                                                 | 0.43              | 0.54       | 2.61                        |
| —CHF <sub>2</sub>                                                |                   |            | 2.05                        |
| —CH <sub>2</sub> F                                               |                   |            | 1.10                        |
| —CH <sub>2</sub> CF <sub>3</sub>                                 |                   |            | 0.90                        |
| —CH <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> |                   |            | 0.87                        |
| —C <sub>6</sub> F <sub>5</sub>                                   | —0.12             | —0.03      |                             |
| —Ge(CH <sub>3</sub> ) <sub>3</sub>                               |                   | 0.0        |                             |
| —Ge(CH <sub>2</sub> CH <sub>3</sub> ) <sub>3</sub>               |                   | 0.0        |                             |
| —H                                                               | 0.00              | 0.00       | 0.49                        |
| —I                                                               | 0.35              | 0.28       | 2.46                        |
| —CH <sub>2</sub> I                                               |                   |            | 0.85                        |
| —IO <sub>2</sub>                                                 | 0.70              | 0.76       |                             |
| —N <sub>2</sub> <sup>+</sup>                                     | 1.76              | 1.91       |                             |
| —N <sub>3</sub> (azide)                                          | 0.33              | 0.08       | 2.62                        |
| —NH <sub>2</sub>                                                 | —0.16             | —0.66      | 0.62                        |
| —NH <sub>3</sub> <sup>+</sup>                                    | 1.13              | 1.70       | 3.76                        |
| —CH <sub>2</sub> —NH <sub>2</sub>                                |                   |            | 0.50                        |
| —CH <sub>2</sub> —NH <sub>3</sub> <sup>+</sup>                   |                   |            | 2.24                        |
| —NH—CH <sub>3</sub>                                              | —0.30             | —0.84      |                             |
| —NH—C <sub>2</sub> H <sub>5</sub>                                | —0.24             | —0.61      |                             |
| —NH—C <sub>4</sub> H <sub>9</sub>                                | —0.34             | —0.51      |                             |
| —NH(CH <sub>3</sub> ) <sub>2</sub> <sup>+</sup>                  |                   |            | 4.36                        |
| —NH <sub>2</sub> —CH <sub>3</sub> <sup>+</sup>                   | 0.96              |            | 3.74                        |
| —NH <sub>2</sub> —C <sub>2</sub> H <sub>5</sub> <sup>+</sup>     | 0.96              |            | 3.74                        |
| —N(CH <sub>3</sub> ) <sub>3</sub> <sup>+</sup>                   | 0.88              | 0.82       | 4.55                        |
| —N(CH <sub>3</sub> ) <sub>2</sub>                                | —0.2              | —0.83      | 0.32                        |
| —CH <sub>2</sub> —N(CH <sub>3</sub> ) <sub>3</sub> <sup>+</sup>  |                   |            | 1.90                        |
| —N(CF <sub>3</sub> ) <sub>2</sub>                                | 0.45              | 0.53       |                             |
| <i>p</i> -H <sub>2</sub> N—C <sub>6</sub> H <sub>5</sub> —       |                   | —0.30      |                             |
| —NH—CO—CH <sub>3</sub>                                           | 0.21              | 0.00       | 1.40                        |
| —NH—CO—C <sub>2</sub> H <sub>5</sub>                             |                   |            | 1.56                        |
| —NH—CO—C <sub>6</sub> H <sub>5</sub>                             | 0.22              | 0.08       | 1.68                        |
| —NH—CHO                                                          | 0.25              |            | 1.62                        |
| —NH—CO—NH <sub>2</sub>                                           | 0.18              |            | 1.31                        |
| —NH—OH                                                           | —0.04             | —0.34      |                             |
| —NH—CO—OC <sub>2</sub> H <sub>5</sub>                            | 0.33              |            | 1.99                        |
| —CH <sub>2</sub> —NH—CO—CH <sub>3</sub>                          |                   |            | 0.43                        |
| —NH—SO <sub>2</sub> —C <sub>6</sub> H <sub>5</sub>               |                   |            | 1.99                        |
| —NH—NH <sub>2</sub>                                              | —0.02             | —0.55      |                             |
| —CN                                                              | 0.56              | 0.66       | 3.30                        |
| —CH <sub>2</sub> —CN                                             | 0.17              | 0.01       | 1.30                        |
| —NO                                                              |                   | 0.12       |                             |
| —NO <sub>2</sub>                                                 | 0.71              | 0.78       | 4.0                         |
| —CH <sub>2</sub> —NO <sub>2</sub>                                |                   |            | 1.40                        |

**TABLE 9.1** Hammett and Taft Substituent Constants (*Continued*)

| Substituent                                                              | Hammett constants |            | Taft constant<br>$\sigma^*$ |
|--------------------------------------------------------------------------|-------------------|------------|-----------------------------|
|                                                                          | $\sigma_m$        | $\sigma_p$ |                             |
| —CH <sub>2</sub> —CH <sub>2</sub> —NO <sub>2</sub>                       |                   |            | 0.50                        |
| —CH=CHNO <sub>2</sub>                                                    | 0.33              | 0.26       |                             |
| <i>m</i> -O <sub>2</sub> N—C <sub>6</sub> H <sub>4</sub>                 |                   | 0.18       |                             |
| <i>p</i> -O <sub>2</sub> N—C <sub>6</sub> H <sub>4</sub>                 |                   | 0.24       |                             |
| (NO <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> — (picryl) | 0.43              | 0.41       |                             |
| —N(CO—CH <sub>3</sub> )(CO—C <sub>6</sub> H <sub>5</sub> )               |                   |            | 1.37                        |
| —N(CO—CH <sub>3</sub> )(naphthyl)                                        |                   |            | 1.65                        |
| —O <sup>−</sup>                                                          | −0.71             | −0.52      |                             |
| —OH                                                                      | 0.12              | −0.37      | 1.34                        |
| —O—CH <sub>3</sub>                                                       | 0.12              | −0.27      | 1.81                        |
| —O—C <sub>2</sub> H <sub>5</sub>                                         | 0.10              | −0.24      | 1.68                        |
| —O—C <sub>3</sub> H <sub>7</sub>                                         | 0.00              | −0.25      | 1.68                        |
| —O—CH(CH <sub>3</sub> ) <sub>2</sub>                                     | 0.05              | −0.45      | 1.62                        |
| —O—C <sub>4</sub> H <sub>9</sub>                                         | −0.05             | −0.32      | 1.68                        |
| —O—cyclopentyl                                                           |                   |            | 1.62                        |
| —O—cyclohexyl                                                            | 0.29              |            | 1.81                        |
| —O—CH <sub>2</sub> —cyclohexyl                                           | 0.18              |            | 1.31                        |
| —O—C <sub>6</sub> H <sub>5</sub>                                         | 0.25              | −0.32      | 2.43                        |
| —O—CH <sub>2</sub> —C <sub>6</sub> H <sub>5</sub>                        |                   | −0.42      |                             |
| —OCF <sub>3</sub>                                                        | 0.40              | 0.35       |                             |
| 3,4-O—CH <sub>2</sub> —O—                                                |                   | −0.27      |                             |
| 3,4-O—(CH <sub>2</sub> —) <sub>2</sub> O—                                |                   | −0.12      |                             |
| —O—CO—CH <sub>3</sub>                                                    | 0.39              | 0.31       |                             |
| —ONO <sub>2</sub>                                                        |                   |            | 3.86                        |
| —O—N=C(CH <sub>3</sub> ) <sub>2</sub>                                    |                   |            | 1.81                        |
| —ONH <sub>3</sub> <sup>+</sup>                                           |                   |            | 2.92                        |
| —CH <sub>2</sub> —O <sup>−</sup>                                         |                   |            | 0.27                        |
| —CH <sub>2</sub> —OH                                                     | 0.08              | 0.08       | 0.31                        |
| —CH <sub>2</sub> —O—CH <sub>3</sub>                                      |                   |            | 0.52                        |
| —CH(OH)—CH <sub>3</sub>                                                  |                   |            | 0.12                        |
| —CH(OH)—C <sub>6</sub> H <sub>5</sub>                                    |                   |            | 0.50                        |
| <i>p</i> -HO—C <sub>6</sub> H <sub>4</sub> —                             |                   | −0.24      |                             |
| <i>p</i> -CH <sub>3</sub> O—C <sub>6</sub> H <sub>4</sub> —              |                   | −0.10      |                             |
| —CH <sub>2</sub> —CH(OH)—CH <sub>3</sub>                                 |                   |            | −0.06                       |
| —CH <sub>2</sub> —C(OH)(CH <sub>3</sub> ) <sub>2</sub>                   |                   |            | −0.25                       |
| —P(CH <sub>3</sub> ) <sub>2</sub>                                        | 0.1               | 0.05       |                             |
| —P(CH <sub>3</sub> ) <sub>3</sub> <sup>+</sup>                           | 0.8               | 0.9        |                             |
| —P(CF <sub>3</sub> ) <sub>2</sub>                                        | 0.6               | 0.7        |                             |
| —PO <sub>3</sub> H <sup>−</sup>                                          | 0.2               | 0.26       |                             |
| —PO(OC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>                        | 0.55              | 0.60       |                             |
| —SH                                                                      | 0.25              | 0.15       | 1.68                        |
| —SCH <sub>3</sub>                                                        | 0.15              | 0.00       | 1.56                        |
| —S(CH <sub>3</sub> ) <sub>2</sub> <sup>+</sup>                           | 1.0               | 0.9        |                             |
| —SCH <sub>2</sub> CH <sub>3</sub>                                        | 0.23              | 0.03       | 1.56                        |
| —SCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>                        |                   |            | 1.49                        |
| —SCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>        |                   |            | 1.44                        |
| —S—cyclohexyl                                                            |                   |            | 1.93                        |
| —SC <sub>6</sub> H <sub>5</sub>                                          | 0.30              |            | 1.87                        |
| —SC(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>                         |                   |            | 0.69                        |
| —SCH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>                          |                   |            | 1.56                        |
| —SCH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>          |                   |            | 1.44                        |
| —CH <sub>2</sub> SH                                                      | 0.03              |            | 0.62                        |

TABLE 9.1 Hammett and Taft Substituent Constants (Continued)

| Substituent                                                             | Hammett constants |            | Taft constant<br>$\sigma^*$ |
|-------------------------------------------------------------------------|-------------------|------------|-----------------------------|
|                                                                         | $\sigma_m$        | $\sigma_p$ |                             |
| —CH <sub>2</sub> SCH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>         |                   |            | 0.37                        |
| —SCF <sub>3</sub>                                                       | 0.40              | 0.50       |                             |
| —SCN                                                                    | 0.63              | 0.52       | 3.43                        |
| —S—CO—CH <sub>3</sub>                                                   | 0.39              | 0.44       |                             |
| —S—CONH <sub>2</sub>                                                    | 0.34              |            | 2.07                        |
| —SO—CH <sub>3</sub>                                                     | 0.52              | 0.49       |                             |
| —SO—C <sub>6</sub> H <sub>5</sub>                                       |                   |            | 3.24                        |
| —CH <sub>2</sub> —SO—CH <sub>3</sub>                                    |                   |            | 1.33                        |
| —SO <sub>2</sub> —CH <sub>3</sub>                                       | 0.60              | 0.68       | 3.68                        |
| —SO <sub>2</sub> —CH <sub>2</sub> CH <sub>3</sub>                       |                   |            | 3.74                        |
| —SO <sub>2</sub> —CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>       |                   |            | 3.68                        |
| —SO <sub>2</sub> —C <sub>6</sub> H <sub>5</sub>                         | 0.67              |            | 3.55                        |
| —SO <sub>2</sub> —CF <sub>3</sub>                                       | 0.79              | 0.93       |                             |
| —SO <sub>2</sub> —NH <sub>2</sub>                                       | 0.46              | 0.57       |                             |
| —CH <sub>2</sub> —SO <sub>2</sub> —CH <sub>3</sub>                      |                   |            | 1.38                        |
| —SO <sub>3</sub>                                                        | 0.05              | 0.09       | 0.81                        |
| —SO <sub>3</sub> H                                                      |                   | 0.50       |                             |
| —SeCH <sub>3</sub>                                                      | 0.1               | 0.0        |                             |
| —Se—cyclohexyl                                                          |                   |            | 2.37                        |
| —SeCN                                                                   | 0.67              | 0.66       | 3.61                        |
| —Si(CH <sub>3</sub> ) <sub>3</sub>                                      | −0.04             | −0.07      | −0.81                       |
| —Si(CH <sub>2</sub> CH <sub>3</sub> ) <sub>3</sub>                      |                   | 0.0        |                             |
| —Si(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>        |                   |            | −0.87                       |
| —Si(CH <sub>3</sub> ) <sub>2</sub> —O—Si(CH <sub>3</sub> ) <sub>3</sub> |                   |            | −0.81                       |
| —CH <sub>2</sub> Si(CH <sub>3</sub> ) <sub>3</sub>                      | −0.16             | −0.22      | −0.25                       |
| —CH <sub>2</sub> CH <sub>2</sub> Si(CH <sub>3</sub> ) <sub>3</sub>      |                   |            | −0.25                       |
| —Sn(CH <sub>3</sub> ) <sub>3</sub>                                      |                   | 0.0        |                             |
| —Sn(CH <sub>2</sub> CH <sub>3</sub> ) <sub>3</sub>                      |                   | 0.0        |                             |

TABLE 9.2  $pK_a^\circ$  and Rho Values for Hammett Equation

| Acid                                                                                | $pK_a^\circ$ | $\rho$ |
|-------------------------------------------------------------------------------------|--------------|--------|
| Arenearsonic acids                                                                  |              |        |
| $pK_1$                                                                              | 3.54         | 1.05   |
| $pK_2$                                                                              | 8.49         | 0.87   |
| Areneboronic acids (in aqueous 25% ethanol)                                         | 9.70         | 2.15   |
| Arenephosphonic acids                                                               |              |        |
| $pK_1$                                                                              | 1.84         | 0.76   |
| $pK_2$                                                                              | 6.97         | 0.95   |
| $\alpha$ -Aryladoximes                                                              | 10.70        | 0.86   |
| Benzeneseleninic acids                                                              | 4.78         | 1.03   |
| Benzenesulfonamides (20°C)                                                          | 10.00        | 1.06   |
| Benzenesulfonanilides (20°C)                                                        |              |        |
| X—C <sub>6</sub> H <sub>4</sub> —SO <sub>2</sub> —NH—C <sub>6</sub> H <sub>5</sub>  | 8.31         | 1.16   |
| C <sub>6</sub> H <sub>5</sub> —SO <sub>2</sub> —NH—C <sub>6</sub> H <sub>4</sub> —X | 8.31         | 1.74   |
| Benzoic acids                                                                       | 4.21         | 1.00   |
| Cinnamic acids                                                                      | 4.45         | 0.47   |
| Phenols                                                                             | 9.92         | 2.23   |



**TABLE 9.2**  $pK_a^\circ$  and Rho Values for Hammett Equation (*Continued*)

| Acid                                              | $pK_a^\circ$ | $\rho$ |
|---------------------------------------------------|--------------|--------|
| Phenylacetic acids                                | 4.30         | 0.49   |
| Phenylpropionic acids (in aqueous 35% dioxane)    | 3.24         | 0.81   |
| Phenylpropionic acids                             | 4.45         | 0.21   |
| Phenyltrifluoromethylcarbinols                    | 11.90        | 1.01   |
| Pyridine-1-oxides                                 | 0.94         | 2.09   |
| 2-Pyridones                                       | 11.65        | 4.28   |
| 4-Pyridones                                       | 11.12        | 4.28   |
| Pyrroles                                          | 17.00        | 4.28   |
| 5-Substituted pyrrole-2-carboxylic acids          | 2.82         | 1.40   |
| Thiobenzoic acids                                 | 2.61         | 1.0    |
| Thiophenols                                       | 6.50         | 2.2    |
| Trifluoroacetophenone hydrates                    | 10.00        | 1.11   |
| 5-Substituted topolones                           | 6.42         | 3.10   |
| <b>Protonated cations of</b>                      |              |        |
| Acetophenones                                     | -6.0         | 2.6    |
| Anilines                                          | 4.60         | 2.90   |
| C-Aryl-N-dibutylamidines (in aqueous 50% ethanol) | 11.14        | 1.41   |
| N,N-Dimethylanilines                              | 5.07         | 3.46   |
| Isoquinolines                                     | 5.32         | 5.90   |
| 1-Naphthylamines                                  | 3.85         | 2.81   |
| 2-Naphthylamines                                  | 4.29         | 2.81   |
| Pyridines                                         | 5.18         | 5.90   |
| Quinolines                                        | 4.88         | 5.90   |

**TABLE 9.3**  $pK_a^\circ$  and Rho Values for Taft Equation

| Acid                                                                                  | $pK_a^\circ$ | $\rho$ |
|---------------------------------------------------------------------------------------|--------------|--------|
| RCOOH                                                                                 | 4.66         | 1.62   |
| RCH <sub>2</sub> COOH                                                                 | 4.76         | 0.67   |
| RC $\equiv$ C—COOH                                                                    | 2.39         | 1.89   |
| H <sub>2</sub> C=C(R)—COOH                                                            | 4.39         | 0.64   |
| (CH <sub>3</sub> ) <sub>2</sub> C=C(R)—COOH                                           | 4.65         | 0.47   |
| <i>cis</i> -C <sub>6</sub> H <sub>5</sub> —CH=C(R)—COOH                               | 3.77         | 0.63   |
| <i>trans</i> -C <sub>6</sub> H <sub>5</sub> —CH=C(R)—COOH                             | 4.61         | 0.47   |
| R—CO—CH <sub>2</sub> —COOH                                                            | 4.12         | 0.43   |
| HON=C(R)—COOH                                                                         | 4.84         | 0.34   |
| RCH <sub>2</sub> OH                                                                   | 15.9         | 1.42   |
| RCH(OH) <sub>2</sub>                                                                  | 14.4         | 1.42   |
| R <sub>1</sub> CO—NHR <sub>2</sub>                                                    | 22.0         | 3.1*   |
| CH <sub>3</sub> CO—C(R)=C(OH)CH <sub>3</sub>                                          | 9.25         | 1.78   |
| CH <sub>3</sub> CO—CH(R)—CO—OC <sub>2</sub> H <sub>5</sub>                            | 12.59        | 3.44   |
| R—CO—NHOH                                                                             | 9.48         | 0.98   |
| R <sub>1</sub> R <sub>2</sub> C=NOH (R <sub>1</sub> , R <sub>2</sub> not acyl groups) | 12.35        | 1.18   |
| (R)(CH <sub>3</sub> CO)C=NOH                                                          | 9.00         | 0.94   |
| RC(NO <sub>2</sub> ) <sub>2</sub> H                                                   | 5.24         | 3.60   |
| RSH                                                                                   | 10.22        | 3.50   |
| RCH <sub>2</sub> SH                                                                   | 10.54        | 1.47   |
| R—CO—SH                                                                               | 3.52         | 1.62   |

TABLE 9.3  $pK_a^\circ$  and Rho Values for Taft Equation (Continued)

| Acid                         | $pK_a^\circ$ | $\rho$ |
|------------------------------|--------------|--------|
| <b>Protonated cations of</b> |              |        |
| $RNH_2$                      | 10.15        | 3.14   |
| $R_1R_2NH$                   | 10.59        | 3.23   |
| $R_1R_2R_3N$                 | 9.61         | 3.30   |
| $R_1R_2PH$                   | 3.59         | 2.61   |
| $R_1R_2R_3P$                 | 7.85         | 2.67   |

\*  $\sigma^*$  for  $R_1CO$  and  $R_2$ .

Two modified sigma constants have been formulated for situations in which the substituent enters into resonance with the reaction center in an electron-demanding transition state ( $\sigma^+$ ) or for an electron-rich transition state ( $\sigma^-$ ).  $\sigma^-$  constants give better correlations in reactions involving phenols, anilines, and pyridines and in nucleophilic substitutions. Values of some modified sigma constants are given in Table 9.4.

TABLE 9.4 Special Hammett Sigma Constants

| Substituent                          | $\sigma_m^+$ | $\sigma_p^+$ | $\sigma_p^-$ |
|--------------------------------------|--------------|--------------|--------------|
| $-\text{CH}_3$                       | -0.07        | -0.31        | -0.17        |
| $-\text{C}(\text{CH}_3)_3$           | -0.06        | -0.26        |              |
| $-\text{C}_6\text{H}_5$              | 0.11         | -0.18        |              |
| $-\text{CF}_3$                       | 0.52         | 0.61         | 0.74         |
| $-\text{F}$                          | 0.35         | -0.07        | 0.02         |
| $-\text{Cl}$                         | 0.40         | 0.11         | 0.23         |
| $-\text{Br}$                         | 0.41         | 0.15         | 0.26         |
| $-\text{I}$                          | 0.36         | 0.14         |              |
| $-\text{CN}$                         | 0.56         | 0.66         | 0.88         |
| $-\text{CHO}$                        |              |              | 1.13         |
| $-\text{CONH}_2$                     |              |              | 0.63         |
| $-\text{COCH}_3$                     |              |              | 0.85         |
| $-\text{COOH}$                       | 0.32         | 0.42         | 0.73         |
| $-\text{CO}-\text{OCH}_3$            | 0.37         | 0.49         | 0.66         |
| $-\text{CO}-\text{OCH}_2\text{CH}_3$ | 0.37         | 0.48         | 0.68         |
| $-\text{N}_2^+$                      |              |              | 3.2          |
| $-\text{NH}_2$                       | 0.16         | -1.3         | -0.66        |
| $-\text{N}(\text{CH}_3)_2$           |              | -1.7         |              |
| $-\text{N}(\text{CH}_3)_3^+$         | 0.36         | 0.41         |              |
| $-\text{NH}-\text{CO}-\text{CH}_3$   |              | -0.60        |              |
| $-\text{NO}_2$                       | 0.67         | 0.79         | 1.25         |
| $-\text{OH}$                         |              | -0.92        |              |
| $-\text{O}^-$                        |              |              | -0.81        |
| $-\text{OCH}_3$                      | 0.05         | -0.78        | -0.27        |
| $-\text{SF}_5$                       |              |              | 0.70         |
| $-\text{SCF}_3$                      |              |              | 0.57         |
| $-\text{SO}_2\text{CH}_3$            |              |              | 1.05         |
| $-\text{SO}_2\text{CF}_3$            |              |              | 1.36         |

---

## SECTION 10

---

# POLYMERS, RUBBERS, FATS, OILS, AND WAXES

---

|         |                                                  |       |
|---------|--------------------------------------------------|-------|
| 10.1    | POLYMERS                                         | 10.2  |
| 10.2    | ADDITIVES TO POLYMERS                            | 10.4  |
| 10.2.1  | Antioxidants                                     | 10.4  |
| 10.2.2  | Antistatic Agents                                | 10.4  |
| 10.2.3  | Chain-Transfer Agents                            | 10.4  |
| 10.2.4  | Coupling Agents                                  | 10.4  |
| 10.2.5  | Flame Retardants                                 | 10.5  |
| 10.2.6  | Foaming Agents (Chemical Blowing Agents)         | 10.5  |
| 10.2.7  | Inhibitors                                       | 10.6  |
| 10.2.8  | Lubricants                                       | 10.6  |
|         | Table 10.1 Plastic Families                      | 10.6  |
| 10.2.9  | Plasticizers                                     | 10.7  |
| 10.2.10 | Ultraviolet Stabilizers                          | 10.7  |
| 10.2.11 | Vulcanization and Curing                         | 10.7  |
| 10.3    | FORMULAS AND KEY PROPERTIES OF PLASTIC MATERIALS | 10.8  |
| 10.3.1  | Acetals                                          | 10.8  |
| 10.3.2  | Acrylics                                         | 10.8  |
| 10.3.3  | Alkyds                                           | 10.9  |
| 10.3.4  | Alloys                                           | 10.10 |
| 10.3.5  | Allyls                                           | 10.10 |
| 10.3.6  | Cellulosics                                      | 10.10 |
| 10.3.7  | Epoxy                                            | 10.11 |
| 10.3.8  | Fluorocarbon                                     | 10.12 |
| 10.3.9  | Nitrile Resins                                   | 10.13 |
| 10.3.10 | Melamine Formaldehyde                            | 10.13 |
| 10.3.11 | Phenolics                                        | 10.14 |
| 10.3.12 | Polyamides                                       | 10.14 |
| 10.3.13 | Poly(amide-imide)                                | 10.15 |
| 10.3.14 | Polycarbonate                                    | 10.15 |
| 10.3.15 | Polyester                                        | 10.15 |
| 10.3.16 | Poly(methylpentene)                              | 10.16 |
| 10.3.17 | Polyolefins                                      | 10.16 |
| 10.3.18 | Poly(phenylene Sulfide)                          | 10.17 |
| 10.3.19 | Polyurethane                                     | 10.18 |
| 10.3.20 | Silicones                                        | 10.18 |
| 10.3.21 | Styrenics                                        | 10.19 |
| 10.3.22 | Sulfones                                         | 10.20 |
| 10.3.23 | Thermoplastic Elastomers                         | 10.20 |
| 10.3.24 | Vinyl                                            | 10.20 |
| 10.3.25 | Urea Formaldehyde                                | 10.21 |
|         | Table 10.2 Properties of Commercial Plastics     | 10.22 |
| 10.4    | FORMULAS AND ADVANTAGES OF RUBBERS               | 10.58 |
| 10.4.1  | Gutta Percha                                     | 10.58 |
| 10.4.2  | Natural Rubber                                   | 10.58 |
| 10.4.3  | Chlorosulfonated Polyethylene                    | 10.58 |
| 10.4.4  | Epichlorohydrin                                  | 10.59 |
| 10.4.5  | Nitrile Rubber (NBR, GRN, Buna N)                | 10.59 |

|         |                                                                                        |            |
|---------|----------------------------------------------------------------------------------------|------------|
| 10.2    |                                                                                        | SECTION 10 |
| 10.4.6  | Polyacrylate                                                                           | 10.59      |
| 10.4.7  | cis-Polybutadiene Rubber (BR)                                                          | 10.59      |
| 10.4.8  | Polychloroprene (Neoprene)                                                             | 10.60      |
| 10.4.9  | Ethylene-Propylene-Diene Rubber (EPDM)                                                 | 10.60      |
| 10.4.10 | Polyisobutylene (Butyl Rubber)                                                         | 10.60      |
| 10.4.11 | (Z)-Polyisoprene (Synthetic Natural Rubber)                                            | 10.60      |
| 10.4.12 | Polysulfide Rubbers                                                                    | 10.61      |
| 10.4.13 | Poly(vinyl Chloride) (PVC)                                                             | 10.61      |
| 10.4.14 | Silicone Rubbers                                                                       | 10.61      |
| 10.4.15 | Styrene-Butadiene Rubber (GRS, SBR, Buna S)                                            | 10.61      |
| 10.4.16 | Urethane                                                                               | 10.62      |
|         | Table 10.3 Properties of Natural and Synthetic Rubbers                                 | 10.63      |
| 10.5    | CHEMICAL RESISTANCE                                                                    | 10.64      |
|         | Table 10.4 Resistance of Selected Polymers and Rubbers to Various Chemicals at 20°C    | 10.64      |
| 10.6    | GAS PERMEABILITY                                                                       | 10.66      |
|         | Table 10.5 Gas Permeability Constants ( $10^{10} P$ ) at 25°C for Polymers and Rubbers | 10.66      |
|         | Table 10.6 Vapor Permeability Constants ( $10^{10} P$ ) at 35°C for Polymers           | 10.69      |
| 10.7    | FATS, OILS, AND WAXES                                                                  | 10.69      |
|         | Table 10.7 Constants of Fats and Oils                                                  | 10.69      |
|         | Table 10.8 Constants of Waxes                                                          | 10.72      |

## 10.1 POLYMERS

---

Polymers are mixtures of macromolecules with similar structures and molecular weights that exhibit some average characteristic properties. In some polymers long segments of linear polymer chains are oriented in a regular manner with respect to one another. Such polymers have many of the physical characteristics of crystals and are said to be *crystalline*. Polymers that have polar functional groups show a considerable tendency to be crystalline. Orientation is aided by alignment of dipoles on different chains. Van der Waals' interactions between long hydrocarbon chains may provide sufficient total attractive energy to account for a high degree of regularity within the polymers.

Irregularities such as branch points, comonomer units, and cross-links lead to *amorphous* polymers. They do not have true melting points but instead have glass transition temperatures at which the rigid and glasslike material becomes a viscous liquid as the temperature is raised.

**Elastomers.** Elastomers is a generic name for polymers that exhibit rubberlike elasticity. Elastomers are soft yet sufficiently elastic that they can be stretched several hundred percent under tension. When the stretching force is removed, they retract rapidly and recover their original dimensions.

Polymers that soften or melt and then solidify and regain their original properties on cooling are called *thermoplastic*. A thermoplastic polymer is usually a single strand of linear polymer with few if any cross-links.

**Thermosetting Polymers.** Polymers that soften or melt on warming and then become infusible solids are called *thermosetting*. The term implies that thermal decomposition has not taken place. Thermosetting plastics contain a cross-linked polymer network that extends through the finished article, making it stable to heat and insoluble in organic solvents. Many molded plastics are shaped while molten and are then heated further to become rigid solids of desired shapes.

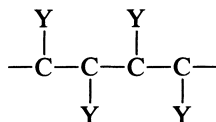
**Synthetic Rubbers.** Synthetic rubbers are polymers with rubberlike characteristics that are prepared from dienes or olefins. Rubbers with special properties can also be prepared from other polymers, such as polyacrylates, fluorinated hydrocarbons, and polyurethanes.

**Structural Differences.** Polymers exhibit structural differences. A *linear* polymer consists of long segments of single strands that are oriented in a regular manner with respect to one another. *Branched* polymers have substituents attached to the repeating units that extend the polymer laterally. When these units participate in chain propagation and link together chains, a *cross-linked* polymer is formed. A *ladder* polymer results when repeating units have a tetravalent structure such that a polymer consists of two backbone chains regularly cross-linked at short intervals.

Generally polymers involve bonding of the most substituted carbon of one monomeric unit to the least substituted carbon atom of the adjacent unit in a *head-to-tail* arrangement. Substituents appear on alternate carbon atoms. *Tacticity* refers to the configuration of substituents relative to the backbone axis. In an *isotactic* arrangement, substituents are on the same plane of the backbone axis; that is, the configuration at each chiral center is identical.

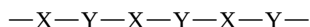


In a *syndiotactic* arrangement, the substituents are in an ordered alternating sequence, appearing alternately on one side and then on the other side of the chain, thus



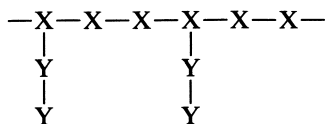
In an *atactic* arrangement, substituents are in an unordered sequence along the polymer chains.

**Copolymerization.** Copolymerization occurs when a mixture of two or more monomer types polymerizes so that each kind of monomer enters the polymer chain. The fundamental structure resulting from copolymerization depends on the nature of the monomers and the relative rates of monomer reactions with the growing polymer chain. A tendency toward alternation of monomer units is common.

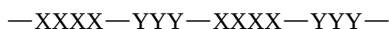


Random copolymerization is rather unusual. Sometimes a monomer which does not easily form a homopolymer will readily add to a reactive group at the end of a growing polymer chain. In turn, that monomer tends to make the other monomer much more reactive.

In *graft copolymers* the chain backbone is composed of one kind of monomer and the branches are made up of another kind of monomer.



The structure of a *block copolymer* consists of a homopolymer attached to chains of another homopolymer.



Configurations around any double bond give rise to *cis* and *trans* stereoisomerism.

## 10.2 ADDITIVES TO POLYMERS

---

### 10.2.1 Antioxidants

Antioxidants markedly retard the rate of autoxidation throughout the useful life of the polymer. Chain-terminating antioxidants have a reactive  $\text{—NH}$  or  $\text{—OH}$  functional group and include compounds such as secondary aryl amines or hindered phenols. They function by transfer of hydrogen to free radicals, principally to peroxy radicals. Butylated hydroxytoluene is a widely used example.

Peroxide-decomposing antioxidants destroy hydroperoxides, the sources of free radicals in polymers. Phosphites and thioesters such as tris(nonylphenyl) phosphite, distearyl pentaerythritol diphosphite, and dialkyl thiodipropionates are examples of peroxide-decomposing antioxidants.

### 10.2.2 Antistatic Agents

External antistatic agents are usually quaternary ammonium salts of fatty acids and ethoxylated glycerol esters of fatty acids that are applied to the plastic surface. Internal antistatic agents are compounded into plastics during processing. Carbon blacks provide a conductive path through the bulk of the plastic. Other types of internal agents must bloom to the surface after compounding in order to be active. These latter materials are ethoxylated fatty amines and ethoxylated glycerol esters of fatty acids, which often must be individually selected to match chemically each plastic type.

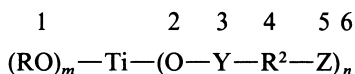
Antistatic agents require ambient moisture to function. Consequently their effectiveness is dependent on the relative humidity. They provide a broad range of protection at 50% relative humidity. Much below 20% relative humidity, only materials which provide a conductive path through the bulk of the plastic to ground (such as carbon black) will reduce electrostatic charging.

### 10.2.3 Chain-Transfer Agents

Chain-transfer agents are used to regulate the molecular weight of polymers. These agents react with the developing polymer and interrupt the growth of a particular chain. The products, however, are free radicals that are capable of adding to monomers and initiating the formation of new chains. The overall effect is to reduce the average molecular weight of the polymer without reducing the rate of polymerization. Branching may occur as a result of chain transfer between a growing but rather short chain with another and longer polymer chain. Branching may also occur if the radical end of a growing chain abstracts a hydrogen from a carbon atom four or five carbons removed from the end. Thiols are commonly used as chain-transfer agents.

### 10.2.4 Coupling Agents

Coupling agents are molecular bridges between the interface of an inorganic surface (or filler) and an organic polymer matrix. Titanium-derived coupling agents interact with the free protons at the inorganic interface to form organic monomolecular layers on the inorganic surface. The titanate-coupling-agent molecule has six functions:



where

| Type       | <i>m</i> | <i>n</i> |
|------------|----------|----------|
| Monoalkoxy | 1        | 3        |
| Coordinate | 4        | 2        |
| Chelate    | 1        | 2        |

Function 1 is the attachment of the hydrolyzable portion of the molecule to the surface of the inorganic (or proton-bearing) species.

Function 2 is the ability of the titanate molecule to transesterify.

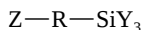
Function 3 affects performance as determined by the chemistry of alkylate, carboxyl, sulfonyl, phenolic, phosphate, pyrophosphate, and phosphite groups.

Function 4 provides van der Waals' entanglement via long carbon chains.

Function 5 provides thermoset reactivity via functional groups such as methacrylates and amines.

Function 6 permits the presence of two or three pendent organic groups. This allows all functionality to be controlled to the first-, second-, or third-degree levels.

Silane coupling agents are represented by the formula



where Y represents a hydrolyzable group (typically alkoxy); Z is a functional organic group, such as amino, methacryloxy, epoxy; and R typically is a small aliphatic linkage that serves to attach the functional organic group to silicon in a stable fashion. Bonding to surface hydroxy groups of inorganic compounds is accomplished by the —SiY<sub>3</sub> portion, either by direct bonding of this group or more commonly via its hydrolysis product —Si(OH)<sub>3</sub>. Subsequent reaction of the functional organic group with the organic matrix completes the coupling reaction and establishes a covalent chemical bond from the organic phase through the silane coupling agent to the inorganic phase.

### 10.2.5 Flame Retardants

Flame retardants are thought to function via several mechanisms, dependent upon the class of flame retardant used. Halogenated flame retardants are thought to function principally in the vapor phase either as a diluent and heat sink or as a free-radical trap that stops or slows flame propagation. Phosphorus compounds are thought to function in the solid phase by forming a glaze or coating over the substrate that prevents the heat and mass transfer necessary for sustained combustion. With some additives, as the temperature is increased, the flame retardant acts as a solvent for the polymer, causing it to melt at lower temperatures and flow away from the ignition source.

Mineral hydrates, such as alumina trihydrate and magnesium sulfate heptahydrate, are used in highly filled thermoset resins.

### 10.2.6 Foaming Agents (Chemical Blowing Agents)

Foaming agents are added to polymers during processing to form minute gas cells throughout the product. Physical foaming agents include liquids and gases. Compressed nitrogen is often used in

injection molding. Common liquid foaming agents are short-chain aliphatic hydrocarbons in the C<sub>5</sub> to C<sub>7</sub> range and their chlorinated or fluorinated analogs.

The chemical foaming agent used varies with the temperature employed during processing. At relatively low temperatures (15 to 200°C), the foaming agent is often 4,4'-oxybis-(benzenesulfonylhydrazide) or *p*-toluenesulfonylhydrazide. In the midrange (160 to 232°C), either sodium hydrogen carbonate or 1,1'-azobisformamide is used. For the high range (200 to 285°C), there are *p*-toluenesulfonyl semicarbazide, 5-phenyltetrazole and analogs, and trihydrazinotriazine.

10.2.7 Inhibitors

Inhibitors slow or stop polymerization by reacting with the initiator or the growing polymer chain. The free radical formed from an inhibitor must be sufficiently unreactive that it does not function as a chain-transfer agent and begin another growing chain. Benzoquinone is a typical free-radical chain inhibitor. The resonance-stabilized free radical usually dimerizes or disproportionates to produce inert products and end the chain process.

10.2.8 Lubricants

Materials such as fatty acids are added to reduce the surface tension and improve the handling qualities of plastic films.

TABLE 10.1 Plastic Families

|                                                                      |                                                                                          |
|----------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Acetals                                                              | Fluorocarbons ( <i>continued</i> )                                                       |
| Acrylics                                                             | Poly(vinylidene fluoride) (PVDF)                                                         |
| Poly(methyl methacrylate) (PMMA)                                     | Ethylene-chlorotrifluoroethylene copolymer                                               |
| Poly(acrylonitrile)                                                  | Ethylene-tetrafluoroethylene copolymer                                                   |
| Alkyds                                                               | Poly(vinyl fluoride) (PVF)                                                               |
| Alloys                                                               | Melamine formaldehyde                                                                    |
| Acrylic-poly(vinyl chloride) alloy                                   | Melamine phenolic                                                                        |
| Acrylonitrile-butadiene-styrene-poly(vinyl chloride) alloy (ABS-PVC) | Nitrile resins                                                                           |
| Acrylonitrile-butadiene-styrene-polycarbonate alloy (ABS-PC)         | Phenolics                                                                                |
| Allyls                                                               | Polyamides                                                                               |
| Allyl-diglycol-carbonate polymer                                     | Nylon 6                                                                                  |
| Diallyl phthalate (DAP) polymer                                      | Nylon 6/6                                                                                |
| Cellulosics                                                          | Nylon 6/9                                                                                |
| Cellulose acetate resin                                              | Nylon 6/12                                                                               |
| Cellulose-acetate-propionate resin                                   | Nylon 11                                                                                 |
| Cellulose-acetate-butyrate resin                                     | Nylon 12                                                                                 |
| Cellulose nitrate resin                                              | Aromatic nylons                                                                          |
| Ethyl cellulose resin                                                | Poly(amide-imide)                                                                        |
| Rayon                                                                | Poly(aryl ether)                                                                         |
| Chlorinated polyether                                                | Polycarbonate (PC)                                                                       |
| Epoxy                                                                | Polyesters                                                                               |
| Fluorocarbons                                                        | Poly(butylene terephthalate) (PBT) [also called polytetramethylene terephthalate (PTMT)] |
| Poly(tetrafluoroethylene) (PTFE)                                     | Poly(ethylene terephthalate) (PET)                                                       |
| Poly(chlorotrifluoroethylene) (PCTFE)                                | Unsaturated polyesters (SMC, BMC)                                                        |
| Perfluoroalkoxy (PFA) resin                                          | Butadiene-maleic acid copolymer (BMC)                                                    |
| Fluorinated ethylene-propylene (FEP) resin                           | Styrene-maleic acid copolymer (SMC)                                                      |
|                                                                      | Polyimide                                                                                |



**TABLE 10.1** Plastic Families (*Continued*)

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Poly(methylpentene)<br>Polyolefins (PO)<br>Low-density polyethylene (LDPE)<br>High-density polyethylene (HDPE)<br>Ultrahigh-molecular-weight polyethylene (UHMWPE)<br>Polypropylene (PP)<br>Polybutylene (PB)<br>Polyallomers<br>Poly(phenylene oxide)<br>Poly(phenylene sulfide) (PPS)<br>Polyurethanes<br>Silicones<br>Styrenics<br>Polystyrene (PS)<br>Acrylonitrile-butadiene-styrene (ABS) copolymer<br>Styrene-acrylonitrile (SAN) copolymer<br>Styrene-butadiene copolymer<br>Sulfones<br>Polysulfone (PSF) | Sulfones ( <i>continued</i> )<br>Poly(ether sulfone)<br>Poly(phenyl sulfone)<br>Thermoplastic elastomers<br>Polyolefin<br>Polyester<br>Block copolymers<br>Styrene-butadiene block copolymer<br>Styrene-isoprene block copolymer<br>Styrene-ethylene block copolymer<br>Styrene-butylene block copolymer<br>Urea formaldehyde<br>Vinyls<br>Poly(vinyl chloride) (PVC)<br>Poly(vinyl acetate) (PVAC)<br>Poly(vinylidene chloride)<br>Poly(vinyl butyrate) (PVB)<br>Poly(vinyl formal)<br>Poly(vinyl alcohol) (PVAL) |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

### 10.2.9 Plasticizers

Plasticizers are relatively nonvolatile liquids which are blended with polymers to alter their properties by intrusion between polymer chains. Diisooctyl phthalate is a common plasticizer. A plasticizer must be compatible with the polymer to avoid bleeding out over long periods of time. Products containing plasticizers tend to be more flexible and workable.

### 10.2.10 Ultraviolet Stabilizers

2-Hydroxybenzophenones represent the largest and most versatile class of ultraviolet stabilizers that are used to protect materials from the degradative effects of ultraviolet radiation. They function by absorbing ultraviolet radiation and by quenching electronically excited states.

Hindered amines, such as 4-(2,2,6,6-tetramethylpiperidinyl) decanedioate, serve as radical scavengers and will protect thin films under conditions in which ultraviolet absorbers are ineffective. Metal salts of nickel, such as dibutyldithiocarbamate, are used in polyolefins to quench singlet oxygen or electronically excited states of other species in the polymer. Zinc salts function as peroxide decomposers.

### 10.2.11 Vulcanization and Curing

Originally, vulcanization implied heating natural rubber with sulfur, but the term is now also employed for curing polymers. When sulfur is employed, sulfide and disulfide cross-links form between polymer chains. This provides sufficient rigidity to prevent *plastic flow*. Plastic flow is a process in which coiled polymers slip past each other under an external deforming force; when the force is released, the polymer chains do not completely return to their original positions.

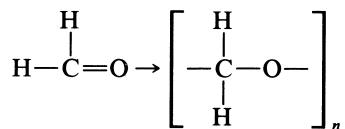
Organic peroxides are used extensively for the curing of unsaturated polyester resins and the polymerization of monomers having vinyl unsaturation. The —O—O— bond is split into free radicals which can initiate polymerization or cross-linking of various monomers or polymers.

### 10.3 FORMULAS AND KEY PROPERTIES OF PLASTIC MATERIALS

---

#### 10.3.1 Acetals

**10.3.1.1 Homopolymer.** Acetal homopolymers are prepared from formaldehyde and consist of high-molecular-weight linear polymers of formaldehyde.



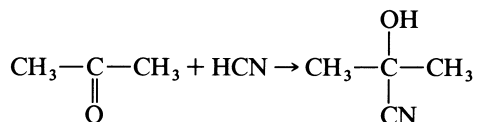
The good mechanical properties of this homopolymer result from the ability of the oxymethylene chains to pack together into a highly ordered crystalline configuration as the polymers change from the molten to the solid state.

Key properties include high melt point, strength and rigidity, good frictional properties, and resistance to fatigue. Higher molecular weight increases toughness but reduces melt flow.

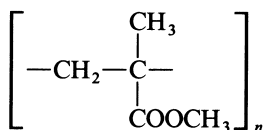
**10.3.1.2 Copolymer.** Acetal copolymers are prepared by copolymerization of 1,3,5-trioxane with small amounts of a comonomer. Carbon-carbon bonds are distributed randomly in the polymer chain. These carbon-carbon bonds help to stabilize the polymer against thermal, oxidative, and acidic attack.

#### 10.3.2 Acrylics

**10.3.2.1 Poly(methyl Methacrylate).** The monomer used for poly(methyl methacrylate), 2-hydroxy-2-methylpropanenitrile, is prepared by the following reaction:

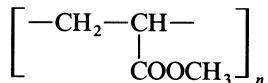


2-Hydroxy-2-methylpropanenitrile is then reacted with methanol (or other alcohol) to yield methacrylate ester. Free-radical polymerization is initiated by peroxide or azo catalysts and produce poly(methyl methacrylate) resins having the following formula:



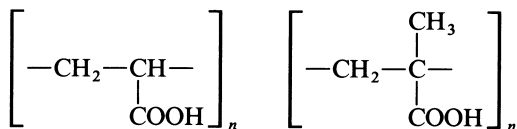
Key properties are improved resistance to heat, light, and weathering. This polymer is unaffected by most detergents, cleaning agents, and solutions of inorganic acids, alkalies, and aliphatic hydrocarbons. Poly(methyl methacrylate) has light transmittance of 92% with a haze of 1 to 3% and its clarity is equal to glass.

**10.3.2.2 Poly(methyl Acrylate).** The monomer used for preparing poly(methyl acrylate) is produced by the oxidation of propylene. The resin is made by free-radical polymerization initiated by peroxide or azo catalysts and has the following formula:



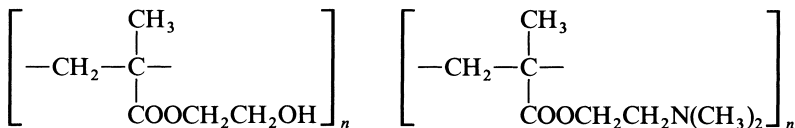
Resins vary from soft, elastic, film-forming materials to hard plastics.

**10.3.2.3 Poly(acrylic Acid) and Poly(methacrylic Acid).** Glacial acrylic acid and glacial methacrylic acid can be polymerized to produce water-soluble polymers having the following structures:



These monomers provide a means for introducing carboxyl groups into copolymers. In copolymers these acids can improve adhesion properties, improve freeze-thaw and mechanical stability of polymer dispersions, provide stability in alkalies (including ammonia), increase resistance to attack by oils, and provide reactive centers for cross-linking by divalent metal ions, diamines, or epoxides.

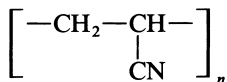
**10.3.2.4 Functional Group Methacrylate Monomers.** Hydroxyethyl methacrylate and dimethylaminoethyl methacrylate produce polymers having the following formulas:



The use of hydroxyethyl (also hydroxypropyl) methacrylate as a monomer permits the introduction of reactive hydroxyl groups into the copolymers. This offers the possibility for subsequent cross-linking with an HO-reactive difunctional agent (diisocyanate, diepoxide, or melamine-formaldehyde resin). Hydroxyl groups promote adhesion to polar substrates.

Use of dimethylaminoethyl (also *tert*-butylaminoethyl) methacrylate as a monomer permits the introduction of pendent amino groups which can serve as sites for secondary cross-linking, provide a way to make the copolymer acid-soluble, and provide anchoring sites for dyes and pigments.

**10.3.2.5 Poly(acrylonitrile).** Poly(acrylonitrile) polymers have the following formula:



### 10.3.3 Alkyds

Alkyds are formulated from polyester resins, cross-linking monomers, and fillers of mineral or glass. The unsaturated polyester resins used for thermosetting alkyds are the reaction products of polyfunctional organic alcohols (glycols) and dibasic organic acids.

Key properties of alkyds are dimensional stability, colorability, and arc track resistance. Chemical resistance is generally poor.

### 10.3.4 Alloys

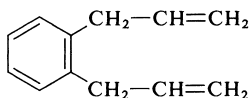
Polymer alloys are physical mixtures of structurally different homopolymers or copolymers. The mixture is held together by secondary intermolecular forces such as dipole interaction, hydrogen bonding, or van der Waals' forces.

Homogeneous alloys have a single glass transition temperature which is determined by the ratio of the components. The physical properties of these alloys are averages based on the composition of the alloy.

Heterogeneous alloys can be formed when graft or block copolymers are combined with a compatible polymer. Alloys of incompatible polymers can be formed if an interfacial agent can be found.

### 10.3.5 Allyls

**10.3.5.1 Diallyl Phthalate (and Diallyl 1,3-Phthalate).** These allyl polymers are prepared from

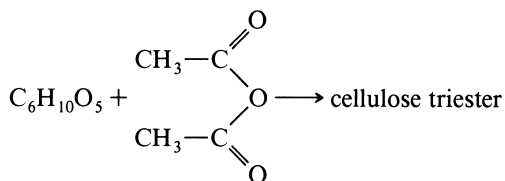


These resulting polymers are solid, linear, internally cyclized, thermoplastic structures containing unreacted allylic groups spaced at regular intervals along the polymer chain.

Molding compounds with mineral, glass, or synthetic fiber filling exhibit good electrical properties under high humidity and high temperature conditions, stable low-loss factors, high surface and volume resistivity, and high arc and track resistance.

### 10.3.6 Cellulosics

**10.3.6.1 Cellulose Triacetate.** Cellulose triacetate is prepared according to the following reaction:



Because cellulose triacetate has a high softening temperature, it must be processed in solution. A mixture of dichloromethane and methanol is a common solvent.

Cellulose triacetate sheeting and film have good gauge uniformity and good optical clarity. Cellulose triacetate products have good dimensional stability and resistance to water and have good folding endurance and burst strength. It is highly resistant to solvents such as acetone. Cellulose triacetate products have good heat resistance and a high dielectric constant.

**10.3.6.2 Cellulose Acetate, Propionate, and Butyrate.** Cellulose acetate is prepared by hydrolyzing the triester to remove some of the acetyl groups; the plastic-grade resin contains 38 to 40%

These cellulose esters form tough, strong, stiff, hard plastics with almost unlimited color possibilities. Articles made from these plastics have a high gloss and are suitable for use in contact with food.

$$\text{C}_6\text{H}_{10}\text{O}_5 + \text{HNO}_3 \rightarrow [-\text{C}_6\text{H}_7\text{O}_2(\text{OH})(\text{ONO}_2)_2-]_n$$

Key properties of cellulose nitrate are good dimensional stability, low water absorption, and toughness. Its disadvantages are its flammability and lack of stability to heat and sunlight.

Although not as resistant as cellulose esters to acids, it is much more resistant to bases. An outstanding feature is its toughness at low temperatures.

**10.3.6.5 Rayon.** Viscose rayon is obtained by reacting the hydroxy groups of cellulose with carbon disulfide in the presence of alkali to give xanthates. When this solution is poured (spun) into an acid medium, the reaction is reversed and the cellulose is regenerated (coagulated).

### 10.3.7 Epoxy

$$\text{CH}_2\text{---CH---CH}_2\text{Cl} + \text{HO---C}_6\text{H}_4\text{---C(CH}_3)_2\text{---C}_6\text{H}_4\text{---OH} \xrightarrow{\text{aq NaOH}}$$

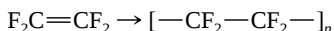
**Bisphenol A**

$$\text{CH}_2\text{---CH---CH}_2\text{---}\left(\text{O---C}_6\text{H}_4\text{---C(CH}_3)_2\text{---C}_6\text{H}_4\text{---O---CH}_2\text{---CH(OH)---CH}_2\right)_n$$

Epoxy novolac resins are produced by glycidation of the low-molecular-weight reaction products of phenol (or cresol) with formaldehyde. Highly cross-linked systems are formed that have superior performance at elevated temperatures.

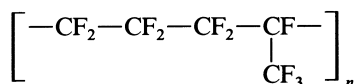
### 10.3.8 Fluorocarbon

**10.3.8.1 Poly(tetrafluoroethylene).** Poly(tetrafluoroethylene) is prepared from tetrafluoroethylene and consists of repeating units in a predominantly linear chain:



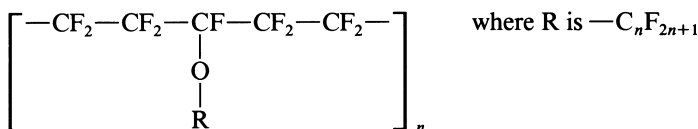
Tetrafluoroethylene polymer has the lowest coefficient of friction of any solid. It has remarkable chemical resistance and a very low brittleness temperature ( $-100^\circ\text{C}$ ). Its dielectric constant and loss factor are low and stable across a broad temperature and frequency range. Its impact strength is high.

**10.3.8.2 Fluorinated Ethylene-Propylene Resin.** Polymer molecules of fluorinated ethylene-propylene consist of predominantly linear chains with this structure:



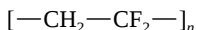
Key properties are its flexibility, translucency, and resistance to all known chemicals except molten alkali metals, elemental fluorine and fluorine precursors at elevated temperatures, and concentrated perchloric acid. It withstands temperatures from  $-270^\circ$  to  $250^\circ\text{C}$  and may be sterilized repeatedly by all known chemical and thermal methods.

**10.3.8.3 Perfluoroalkoxy Resin.** Perfluoroalkoxy resin has the following formula:



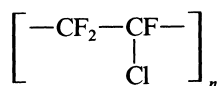
It resembles polytetrafluoroethylene and fluorinated ethylene propylene in its chemical resistance, electrical properties, and coefficient of friction. Its strength, hardness, and wear resistance are about equal to the former plastic and superior to that of the latter at temperatures above  $150^\circ\text{C}$ .

**10.3.8.4 Poly(vinylidene Fluoride).** Poly(vinylidene fluoride) consists of linear chains in which the predominant repeating unit is



It has good weathering resistance and does not support combustion. It is resistant to most chemicals and solvents and has greater strength, wear resistance, and creep resistance than the preceding three fluorocarbon resins.

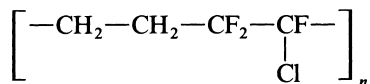
**10.3.8.5 Poly(1-Chloro-1,2,2-Trifluoroethylene).** Poly(1-chloro-1,2,2-trifluoroethylene) consists of linear chains in which the predominant repeating unit is



It possesses outstanding barrier properties to gases, especially water vapor. It is surpassed only by the fully fluorinated polymers in chemical resistance. A few solvents dissolve it at temperatures

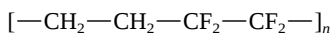
above 100°C, and it is swollen by a number of solvents, especially chlorinated solvents. It is harder and stronger than perfluorinated polymers, and its impact strength is lower.

**10.3.8.6 Ethylene-Chlorotrifluoroethylene Copolymer.** Ethylene-chlorotrifluoroethylene copolymer consists of linear chains in which the predominant 1 : 1 alternating copolymer is



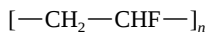
This copolymer has useful properties from cryogenic temperatures to 180°C. Its dielectric constant is low and stable over a broad temperature and frequency range.

**10.3.8.7 Ethylene-Tetrafluoroethylene Copolymer.** Ethylene-tetrafluoroethylene copolymer consists of linear chains in which the repeating unit is



Its properties resemble those of ethylene-chlorotrifluoroethylene copolymer.

**10.3.8.8 Poly(vinyl Fluoride).** Poly(vinyl fluoride) consists of linear chains in which the repeating unit is



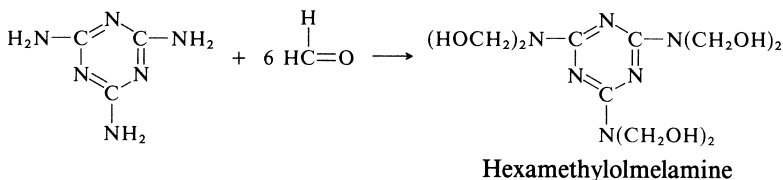
It is used only as a film, and it has good resistance to abrasion and resists staining. It also has outstanding weathering resistance and maintains useful properties from -100 to 150°C.

### 10.3.9 Nitrile Resins

The principal monomer of nitrile resins is acrylonitrile (see “Polyacrylonitrile”), which constitutes about 70% by weight of the polymer and provides the polymer with good gas barrier and chemical resistance properties. The remainder of the polymer is 20 to 30% methylacrylate (or styrene), with 0 to 10% butadiene to serve as an impact-modifying monomer.

### 10.3.10 Melamine Formaldehyde

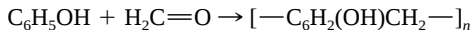
The monomer used for preparing melamine formaldehyde is formed as follows:



Hexamethylolmelamine can further condense in the presence of an acid catalyst; ether linkages can also form (see “Urea Formaldehyde”). A wide variety of resins can be obtained by careful selection of pH, reaction temperature, reactant ratio, amino monomer, and extent of condensation. Liquid coating resins are prepared by reacting methanol or butanol with the initial methylolated products. These can be used to produce hard, solvent-resistant coatings by heating with a variety of hydroxy, carboxyl, and amide functional polymers to produce a cross-linked film.

### 10.3.11 Phenolics

**10.3.11.1 Phenol-Formaldehyde Resin.** Phenol-formaldehyde resin is prepared as follows:

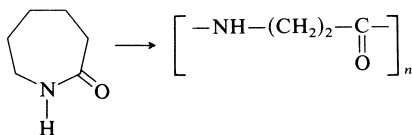


**One-Stage Resins.** The ratio of formaldehyde to phenol is high enough to allow the thermosetting process to take place without the addition of other sources of cross-links.

**Two-Stage Resins.** The ratio of formaldehyde to phenol is low enough to prevent the thermosetting reaction from occurring during manufacture of the resin. At this point the resin is termed *novolac* resin. Subsequently, hexamethylenetetramine is incorporated into the material to act as a source of chemical cross-links during the molding operation (and conversion to the thermoset or cured state).

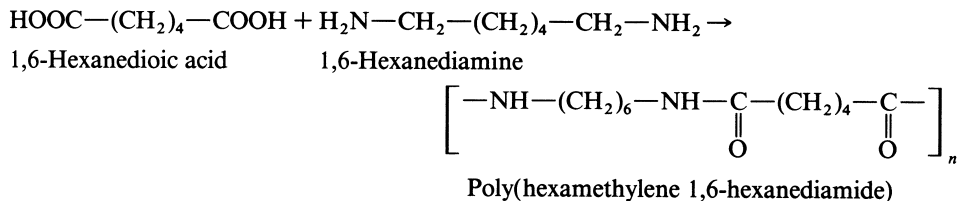
### 10.3.12 Polyamides

**10.3.12.1 Nylon 6, 11, and 12.** This class of polymers is polymerized by addition reactions of ring compounds that contain both acid and amine groups on the monomer.



Nylon 6 is polymerized from 2-oxohexamethyleneimine (6 carbons); nylon 11 and 12 are made this way from 11- and 12-carbon rings, respectively.

**10.3.12.2 Nylon 6/6, 6/9, and 6/12.** As illustrated below, nylon 6/6 is polymerized from 1,6-hexanedioic acid (six carbons) and 1,6-hexanediamine (six carbons).



Other nylons are made this way from direct combinations of monomers to produce types 6/9, 6/10, and 6/12.

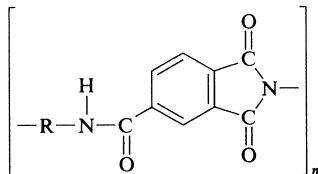
Nylon 6 and 6/6 possess the maximum stiffness, strength, and heat resistance of all the types of nylon. Type 6/6 has a higher melt temperature, whereas type 6 has a higher impact resistance and better processibility. At a sacrifice in stiffness and heat resistance, the higher analogs of nylon are useful primarily for improved chemical resistance in certain environments (acids, bases, and zinc chloride solutions) and for lower moisture absorption.

Aromatic nylons,  $[-\text{NH}-\text{C}_6\text{H}_4-\text{CO}-]_n$  (also called aramids), have specialty uses because of their improved clarity.



### 10.3.13 Poly(amide-imide)

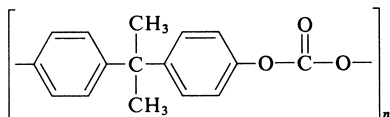
Poly(amide-imide) is the condensation polymer of 1,2,4-benzenetricarboxylic anhydride and various aromatic diamines and has the general structure:



It is characterized by high strength and good impact resistance, and retains its physical properties at temperatures up to 260°C. Its radiation (gamma) resistance is good.

### 10.3.14 Polycarbonate

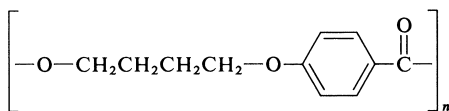
Polycarbonate is a polyester in which dihydric (or polyhydric) phenols are joined through carbonate linkages. The general-purpose type of polycarbonate is based on 2,2-bis(4'-hydroxybenzene)propane (bisphenol A) and has the general structure:



Polycarbonates are the toughest of all thermoplastics. They are window-clear, amazingly strong and rigid, autoclavable, and nontoxic. They have a brittleness temperature of -135°C.

### 10.3.15 Polyester

**10.3.15.1 Poly(butylene Terephthalate).** Poly(butylene terephthalate) is prepared in a condensation reaction between dimethyl terephthalate and 1,4-butanediol and its repeating unit has the general structure



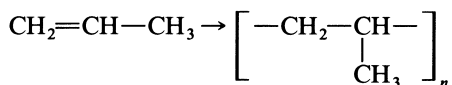
This thermoplastic shows good tensile strength, toughness, low water absorption, and good frictional properties, plus good chemical resistance and electrical properties.

**10.3.15.2 Poly(ethylene Terephthalate).** Poly(ethylene terephthalate) is prepared by the reaction of either terephthalic acid or dimethyl terephthalate with ethylene glycol, and its repeating unit has the general structure.



A key property is its chemical inertness. Strong oxidizing agents eventually cause some oxidation, and some solvents cause softening or swelling, but there is no known solvent for polyethylene at room temperature. The brittleness temperature is  $-100^{\circ}\text{C}$  for both types. Polyethylene has good low-temperature toughness, low water absorption, and good flexibility at subzero temperatures.

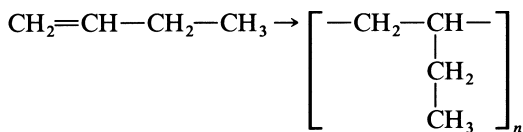
**10.3.17.2 Polypropylene.** The polymerization of propylene results in a polymer with the following structure:



The desired form in homopolymers is the isotactic arrangement (at least 93% is required to give the desired properties). Copolymers have a random arrangement. In block copolymers a secondary reactor is used where active polymer chains can further polymerize to produce segments that use ethylene monomer.

Polypropylene is translucent and autoclavable and has no known solvent at room temperature. It is slightly more susceptible to strong oxidizing agents than polyethylene.

**10.3.17.3 Polybutylene.** Polybutylene is composed of linear chains having an isotactic arrangement of ethyl side groups along the chain backbone.



It has a helical conformation in the stable crystalline form.

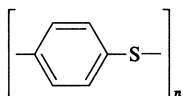
Polybutylene exhibits high tear, impact, and puncture resistance. It also has low creep, excellent chemical resistance, and abrasion resistance with coilability.

**10.3.17.4 Ionomer.** Ionomer is the generic name for polymers based on sodium or zinc salts of ethylene-methacrylic acid copolymers in which interchain ionic bonding, occurring randomly between the long-chain polymer molecules, produces solid-state properties.

The abrasion resistance of ionomers is outstanding, and ionomer films exhibit optical clarity. In composite structures ionomers serve as a heat-seal layer.

### 10.3.18 Poly(phenylene Sulfide)

Poly(phenylene sulfide) has the following formula:

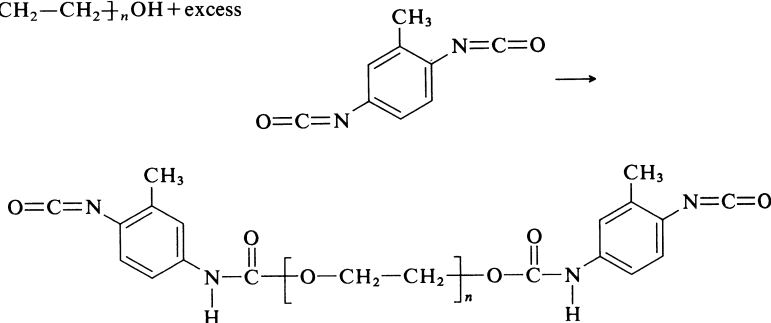


The recurring *para*-substituted benzene rings and sulfur atoms form a symmetrical rigid backbone.

The high degree of crystallization and the thermal stability of the bond between the benzene ring and sulfur are the two properties responsible for the polymer's high melting point, thermal stability, inherent flame retardance, and good chemical resistance. There are no known solvents of poly(phenylene sulfide) that can function below  $205^{\circ}\text{C}$ .

### 10.3.19 Polyurethane

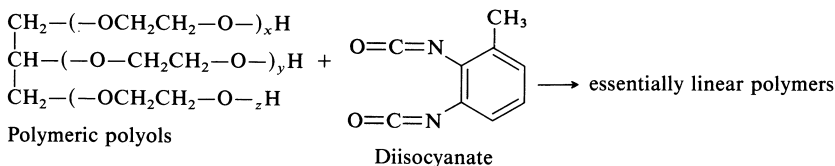
**10.3.19.1 Foams.** Polyurethane foams are prepared by the polymerization of polyols with isocyanates.



Commonly used isocyanates are toluene diisocyanate, methylene diphenyl isocyanate, and polymeric isocyanates. Polyols used are macroglycols based on either polyester or polyether. The former [poly(ethylene phthalate) or poly(ethylene 1,6-hexanedioate)] have hydroxyl groups that are free to react with the isocyanate. Most flexible foam is made from 80/20 toluene diisocyanate (which refers to the ratio of 2,4-toluene diisocyanate to 2,6-toluene diisocyanate). High-resilience foam contains about 80% 80/20 toluene diisocyanate and 20% poly(methylene diphenyl isocyanate), while semi-flexible foam is almost always 100% poly(methylene diphenyl isocyanate). Much of the latter reacts by trimerization to form isocyanurate rings.

Flexible foams are used in mattresses, cushions, and safety applications. Rigid and semiflexible foams are used in structural applications and to encapsulate sensitive components to protect them against shock, vibration, and moisture. Foam coatings are tough, hard, flexible, and chemically resistant.

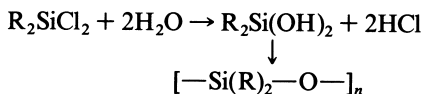
**10.3.19.2 Elastomeric Fiber.** Elastomeric fibers are prepared by the polymerization of polymeric polyols with diisocyanates.



The structure of elastomeric fibers is similar to that illustrated for polyurethane foams.

### 10.3.20 Silicones

Silicones are formed in the following multistage reaction:



The silanols formed above are unstable and under dehydration. On polycondensation, they give polysiloxanes (or silicones) which are characterized by their three-dimensional branched-chain structure. Various organic groups introduced within the polysiloxane chain impart certain characteristics and properties to these resins.

Methyl groups impart water repellency, surface hardness, and noncombustibility.

Phenyl groups impart resistance to temperature variations, flexibility under heat, resistance to abrasion, and compatibility with organic products.

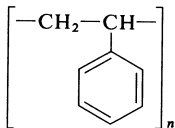
Vinyl groups strengthen the rigidity of the molecular structure by creating easier cross-linkage of molecules.

Methoxy and alkoxy groups facilitate cross-linking at low temperatures.

Oils and gums are nonhighly branched- or straight-chain polymers whose viscosity increases with the degree of polycondensation.

### 10.3.21 Styrenics

**10.3.21.1 Polystyrene.** Polystyrene has the following formula:



Polystyrene is rigid with excellent dimensional stability, has good chemical resistance to aqueous solutions, and is an extremely clear material.

Impact polystyrene contains polybutadiene added to reduce brittleness. The polybutadiene is usually dispersed as a discrete phase in a continuous polystyrene matrix. Polystyrene can be grafted onto rubber particles, which assures good adhesion between the phases.

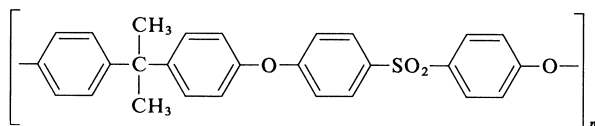
**10.3.21.2 Acrylonitrile-Butadiene-Styrene (ABS) Copolymers.** This basic three-monomer system can be tailored to yield resins with a variety of properties. Acrylonitrile contributes heat resistance, high strength, and chemical resistance. Butadiene contributes impact strength, toughness, and retention of low-temperature properties. Styrene contributes gloss, processibility, and rigidity. ABS polymers are composed of discrete polybutadiene particles grafted with the styrene-acrylonitrile copolymer; these are dispersed in the continuous matrix of the copolymer.

**10.3.21.3 Styrene-Acrylonitrile (SAN) Copolymers.** SAN resins are random, amorphous copolymers whose properties vary with molecular weight and copolymer composition. An increase in molecular weight or in acrylonitrile content generally enhances the physical properties of the copolymer but at some loss in ease of processing and with a slight increase in polymer color.

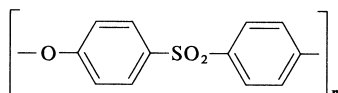
SAN resins are rigid, hard, transparent thermoplastics which process easily and have good dimensional stability—a combination of properties unique in transparent polymers.

### 10.3.22 Sulfones

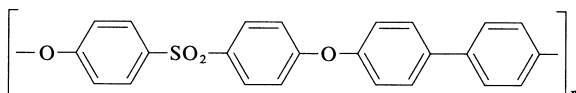
Below are the formulas for three polysulfones.



Polysulfone



Poly(ester sulfone)



Poly(phenyl sulfone)

The isopropylidene linkage imparts chemical resistance, the ether linkage imparts temperature resistance, and the sulfone linkage imparts impact strength. The brittleness temperature of polysulfones is  $-100^\circ\text{C}$ . Polysulfones are clear, strong, nontoxic, and virtually unbreakable. They do not hydrolyze during autoclaving and are resistant to acids, bases, aqueous solutions, aliphatic hydrocarbons, and alcohols.

### 10.3.23 Thermoplastic Elastomers

**10.3.23.1 Polyolefins.** In these thermoplastic elastomers the hard component is a crystalline polyolefin, such as polyethylene or polypropylene, and the soft portion is composed of ethylene-propylene rubber. Attractive forces between the rubber and resin phases serve as labile cross-links. Some contain a chemically cross-linked rubber phase that imparts a higher degree of elasticity.

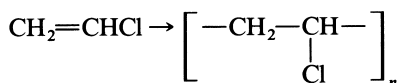
**10.3.23.2 Styrene-Butadiene-Styrene Block Copolymers.** Styrene blocks associate into domains that form hard regions. The midblock, which is normally butadiene, ethylene-butene, or isoprene blocks, forms the soft domains. Polystyrene domains serve as cross-links.

**10.3.23.3 Polyurethanes.** The hard portion of polyurethane consists of a chain extender and polyisocyanate. The soft component is composed of polyol segments.

**10.3.23.4 Polyesters.** The hard portion consists of copolyester, and the soft portion is composed of polyol segments.

### 10.3.24 Vinyl

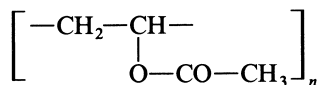
**10.3.24.1 Poly(vinyl Chloride) (PVC).** Polymerization of vinyl chloride results in the formation of a polymer with the following formula:



When blended with phthalate ester plasticizers, PVC becomes soft and pliable.

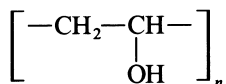
Its key properties are good resistance to oils and a very low permeability to most gases.

**10.3.24.2 Poly(vinyl Acetate).** Poly(vinyl acetate) has the following formula:



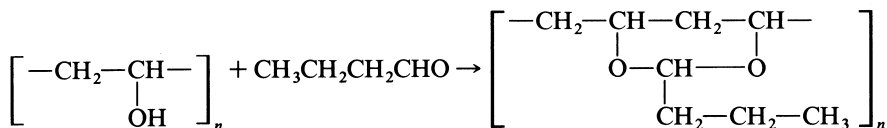
Poly(vinyl acetate) is used in latex water paints because of its weathering, quick-drying, recoatability, and self-priming properties. It is also used in hot-melt and solution adhesives.

**10.3.24.3 Poly(vinyl Alcohol).** Poly(vinyl alcohol) has the following formula:



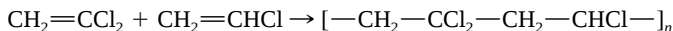
It is used in adhesives, paper coating and sizing, and textile warp size and finishing applications.

**10.3.24.4 Poly(vinyl Butyral).** Poly(vinyl butyral) is prepared according to the following reaction:



Its key characteristics are its excellent optical and adhesive properties. It is used as the interlayer film for safety glass.

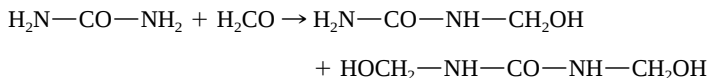
**10.3.24.5 Poly(vinylidene Chloride).** Poly(vinylidene chloride) is prepared according to the following reaction:



Random copolymer

### 10.3.25 Urea Formaldehyde

The reaction of urea with formaldehyde yields the following products, which are used as monomers in the preparation of urea formaldehyde resin.



The reaction conditions can be varied so that only one of those monomers is formed. 1-Hydroxymethylurea and 1,3-bis(hydroxymethyl)urea condense in the presence of an acid catalyst to produce urea formaldehyde resins. A wide variety of resins can be obtained by careful selection of the pH, reaction temperature, reactant ratio, amino monomer, and degree of polymerization. If the reaction is carried far enough, an infusible polymer network is produced.

Liquid coating resins are prepared by reacting methanol or butanol with the initial hydroxymethylureas. Ether exchange reactions between the amino resin and the reactive sites on the polymer produce a cross-linked film.

**TABLE 10.2** Properties of Commercial Plastics

| Properties                                                    | Acetal           |                  |                                  |                                |                                                  |
|---------------------------------------------------------------|------------------|------------------|----------------------------------|--------------------------------|--------------------------------------------------|
|                                                               | Homopolymer      | Copolymer        | 20% glass-reinforced homopolymer | 25% glass-reinforced copolymer | 21% poly(tetrafluoroethylene)-filled homopolymer |
| <u>Physical</u>                                               |                  |                  |                                  |                                |                                                  |
| Melting temperature, °C                                       |                  |                  |                                  |                                |                                                  |
| Crystalline                                                   | 175              | 175              | 181                              | 175                            | 181                                              |
| Amorphous                                                     |                  |                  |                                  |                                |                                                  |
| Specific gravity                                              | 1.42             | 1.41             | 1.56                             | 1.61                           | 1.54                                             |
| Water absorption (24 h), %                                    | 0.25–0.40        | 0.22             | 0.25                             | 0.29                           | 0.20                                             |
| Dielectric strength, KV · mm <sup>-1</sup>                    | 19.7             | 19.7             | 19.3                             | 22.8                           | 15.7                                             |
| <u>Electrical</u>                                             |                  |                  |                                  |                                |                                                  |
| Volume (dc) resistivity, ohm-cm                               | 10 <sup>15</sup> | 10 <sup>15</sup> | 5 × 10 <sup>14</sup>             |                                | 3 × 10 <sup>16</sup>                             |
| Dielectric constant (60 Hz)                                   | 3.7              | 3.7              | 3.9                              |                                | 3.1                                              |
| Dielectric constant (10 <sup>6</sup> Hz)                      | 3.7              | 3.7              | 3.9                              |                                | 3.1                                              |
| Dissipation (power) factor (60 Hz)                            |                  |                  |                                  |                                |                                                  |
| Dissipation factor (10 <sup>6</sup> Hz)                       | 0.005            | 0.005            | 0.005                            |                                | 0.005                                            |
| <u>Mechanical</u>                                             |                  |                  |                                  |                                |                                                  |
| Compressive modulus,<br>10 <sup>3</sup> lb · in <sup>-2</sup> | 670              | 450              |                                  |                                |                                                  |



**TABLE 10.2** Properties of Commercial Plastics (Continued)

| Properties                                                                       | Acetal      |                |                                  |                                |                                                  |
|----------------------------------------------------------------------------------|-------------|----------------|----------------------------------|--------------------------------|--------------------------------------------------|
|                                                                                  | Homopolymer | Copolymer      | 20% glass-reinforced homopolymer | 25% glass-reinforced copolymer | 21% poly(tetrafluoroethylene)-filled homopolymer |
| Compressive strength, rupture or 1% yield, 10 <sup>3</sup> lb · in <sup>-2</sup> | 5.29        | 16 (10% yield) | 18 (10% yield)                   | 17 (10% yield)                 | 13 (10% yield)                                   |
| Elongation at break, %                                                           | 25–75       | 40–75          | 7                                | 3                              | 15–22                                            |
| Flexural modulus at 23°C, 10 <sup>3</sup> lb · in <sup>2</sup>                   | 380–430     | 375            | 730                              | 1100                           | 340–350                                          |
| Flexural strength, rupture or yield, 10 <sup>3</sup> lb · in <sup>-2</sup>       | 14          | 13             | 15                               | 28                             |                                                  |
| Hardness, Rockwell (or Shore)                                                    | M94         | M78            | M90                              | M79                            | M78                                              |
| Impact strength (Izod) at 23°C, J · m <sup>-1</sup>                              | 69–123      | 53–80          | 43                               | 96                             | 37–64                                            |
| Tensile modulus, 10 <sup>3</sup> lb · in <sup>-2</sup>                           | 520         | 410            | 1000                             | 1250                           |                                                  |
| Tensile strength at break, 10 <sup>3</sup> lb · in <sup>-2</sup>                 | 10          | 10             | 8.5                              | 18.5                           | 7.6                                              |
| Tensile yield strength, 10 <sup>3</sup> lb · in <sup>-2</sup>                    | 9.5–12      | 8.5            |                                  |                                | 6.9–7.6                                          |
| <b>Thermal</b>                                                                   |             |                |                                  |                                |                                                  |
| Burning rate, mm · min <sup>-1</sup>                                             | 27.9        |                |                                  |                                |                                                  |
| Coefficient of linear thermal expansion, 10 <sup>-6</sup> °C                     | 100         | 85             | 36–81                            |                                | 75                                               |
| Deflection temperature under flexural load (264 lb · in <sup>-2</sup> ), °C      | 124         | 110            | 157                              | 163                            | 100                                              |
| Maximum recommended service temperature, °C                                      | 84          |                |                                  |                                |                                                  |
| Specific heat, cal · g <sup>-1</sup>                                             | 0.35        |                |                                  |                                |                                                  |
| Thermal conductivity, W · m <sup>-1</sup> · K <sup>-1</sup>                      | 0.23        | 0.23           |                                  |                                |                                                  |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                    |                              |                    |                     |                    |             | Alloy                                    |                                                                           |
|---------------------------------------------------------------|------------------------------|--------------------|---------------------|--------------------|-------------|------------------------------------------|---------------------------------------------------------------------------|
|                                                               | Acrylic                      |                    |                     |                    |             | Acrylic<br>poly(vinyl<br>chloride) alloy | Acrylonitrile-<br>butadiene-<br>styrene-<br>poly(vinyl<br>chloride) alloy |
|                                                               | Poly(methyl<br>methacrylate) | Cast<br>sheet      | Impact-<br>modified | Heat-<br>resistant |             |                                          |                                                                           |
| <u>Physical</u>                                               |                              |                    |                     |                    |             |                                          |                                                                           |
| Melting temperature, °C                                       |                              |                    |                     |                    |             |                                          |                                                                           |
| Crystalline                                                   | 90–105                       | 90–105             | 80–100              | 100–125            |             | 105                                      |                                                                           |
| Amorphous                                                     |                              |                    |                     |                    |             |                                          |                                                                           |
| Specific gravity                                              | 1.17–1.20                    | 1.18–1.20          | 1.11–1.18           | 1.16–1.19          | 2.22–2.24   |                                          |                                                                           |
| Water absorption (24 h), %                                    | 0.1–0.4                      | 0.2–0.4            | 0.2–0.8             | 0.2–0.3            |             | 0.06                                     |                                                                           |
| Dielectric strength, KV · mm <sup>−1</sup>                    | 15.7–19.9                    | 17.7–21.7          | 15.0–19.9           | 15.7–19.9          |             | > 15.7                                   | 19.7                                                                      |
| <u>Electrical</u>                                             |                              |                    |                     |                    |             |                                          |                                                                           |
| Volume (dc) resistivity, ohm-cm                               | > 10 <sup>14</sup>           | > 10 <sup>14</sup> |                     |                    |             |                                          |                                                                           |
| Dielectric constant (60 Hz)                                   | 3.3–4.5                      | 3.5–4.5            |                     |                    | 3.8–5.0     |                                          |                                                                           |
| Dielectric constant (10 <sup>6</sup> Hz)                      |                              | 3.0–3.5            |                     |                    | 3.6–4.7     |                                          |                                                                           |
| Dissipation (power) factor (60 Hz)                            |                              | 0.04–0.06          |                     |                    | 0.012–0.026 |                                          |                                                                           |
| Dissipation factor (10 <sup>6</sup> Hz)                       |                              | 0.02–0.03          |                     |                    | 0.01–0.016  |                                          |                                                                           |
| <u>Mechanical</u>                                             |                              |                    |                     |                    |             |                                          |                                                                           |
| Compressive modulus,<br>10 <sup>4</sup> lb · in <sup>−2</sup> | 370–460                      | 390–475            | 240–370             | 350–460            |             | 330–400                                  |                                                                           |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                              | Acrylic                      |               |                     |                    | Alkyd,<br>molded       | Alloy                                    |                                                                           |
|---------------------------------------------------------------------------------------------------------|------------------------------|---------------|---------------------|--------------------|------------------------|------------------------------------------|---------------------------------------------------------------------------|
|                                                                                                         |                              |               |                     |                    |                        | Acrylic<br>poly(vinyl<br>chloride) alloy | Acrylonitrile-<br>butadiene-<br>styrene-<br>poly(vinyl<br>chloride) alloy |
|                                                                                                         | Poly(methyl<br>methacrylate) | Cast<br>sheet | Impact-<br>modified | Heat-<br>resistant |                        |                                          |                                                                           |
| Compressive strength, rupture or<br>1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$                    | 12–18                        | 11–19         | 4–14                | 17                 | 16–20                  | 8.4                                      |                                                                           |
| Elongation at break, %                                                                                  | 2–10                         | 2–7           | 20–70               | 3–5                |                        | 100                                      |                                                                           |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                                     | 420–460                      | 390–475       | 200–380             | 460–500            |                        | 330–400                                  | 340                                                                       |
| Flexural strength, rupture or yield,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                          | 13–19                        | 12–17         | 7–13                | 12–16              |                        | 10.7                                     | 9.6                                                                       |
| Hardness, Rockwell (or Shore)                                                                           | M85–M105                     | M80–M100      | R105–R120           | M95–M105           | E76                    | R99–R105                                 | R100                                                                      |
| Impact strength (Izod) at 23°C,<br>$\text{J} \cdot \text{m}^{-1}$                                       | 16–27                        | 16–21         | 43–133              | 16–21              | 27–240                 | 800                                      | 560                                                                       |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                                 | 380–450                      | 350–450       | 200–400             | 350–460            |                        | 330–335                                  | 330                                                                       |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                                    | 7–11                         | 8–11          | 5–9                 | 10                 | 4.5–6.5<br>10–13       | 6.5                                      | 5.8                                                                       |
| Tensile yield strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                                       |                              |               |                     |                    |                        |                                          |                                                                           |
| Thermal                                                                                                 |                              |               |                     |                    |                        |                                          |                                                                           |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                                         |                              | 0.5–2.2       |                     |                    | Self-<br>extinguishing |                                          |                                                                           |
| Coefficient of linear thermal<br>expansion, $10^{-6}/^\circ\text{C}$                                    | 50–90                        | 50–90         | 50–80               | 50–60              | 40–55                  |                                          | 46                                                                        |
| Deflection temperature under<br>flexural load (264 $\text{lb} \cdot \text{in}^{-2}$ ), $^\circ\text{C}$ | 74–99                        | 71–102        | 74–95               | 88–104             | 177–204                | 71                                       |                                                                           |
| Maximum recommended service<br>temperature, $^\circ\text{C}$                                            |                              | 60–71         |                     |                    | 220                    |                                          |                                                                           |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                                         | 0.36                         | 0.35          |                     |                    |                        |                                          |                                                                           |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1}, \text{K}^{-1}$                                  | 0.17–0.25                    | 0.17–0.25     | 0.17–0.21           | 0.19               |                        |                                          |                                                                           |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                    | Alloy                                                          | Allyl                                   |                           |                | Cellulosic                         |                                    |                                          |
|---------------------------------------------------------------|----------------------------------------------------------------|-----------------------------------------|---------------------------|----------------|------------------------------------|------------------------------------|------------------------------------------|
|                                                               | Polycarbonate<br>acrylonitrile-<br>butadiene-<br>styrene alloy | Allyl-diglycol-<br>carbonate<br>polymer | Diallyl phthalate molding |                | Cellulose acetate                  |                                    | Cellulose-<br>acetate-<br>butyrate resin |
|                                                               |                                                                |                                         | Glass-filled              | Mineral-filled | Sheet                              | Molding                            | Sheet                                    |
| <u>Physical</u>                                               |                                                                |                                         |                           |                |                                    |                                    |                                          |
| Melting temperature, °C                                       |                                                                |                                         |                           |                |                                    |                                    |                                          |
| Crystalline                                                   |                                                                | Thermoset                               | Thermoset                 | Thermoset      | 230                                | 230                                | 140                                      |
| Amorphous                                                     | 150                                                            |                                         |                           |                |                                    |                                    |                                          |
| Specific gravity                                              | 1.12–1.20                                                      | 1.3–1.4                                 | 1.7–2.0                   | 1.65–1.85      | 1.27–1.34                          | 1.29–1.34                          | 1.15–1.22                                |
| Water absorption (24 h), %                                    | 0.21–0.24                                                      | 0.2                                     | 0.12–0.35                 | 0.2–0.5        | 2–7                                | 1.7–6.5                            | 0.9–2.2                                  |
| Dielectric strength, kV · mm <sup>-1</sup>                    | 17.7                                                           | 15.0                                    | 15.7–17.7                 | 15.7–17.7      | 11–24                              | 9–24                               | 9–18                                     |
| <u>Electrical</u>                                             |                                                                |                                         |                           |                |                                    |                                    |                                          |
| Volume (dc) resistivity, ohm-<br>cm                           |                                                                |                                         |                           |                | 10 <sup>10</sup> –10 <sup>13</sup> | 10 <sup>10</sup> –10 <sup>13</sup> | 10 <sup>10</sup> –10 <sup>12</sup>       |
| Dielectric constant (60 Hz)                                   |                                                                |                                         |                           |                | 3.4–7.4                            | 3.5–7.5                            | 3.7–4.3                                  |
| Dielectric constant (10 <sup>6</sup> Hz)                      |                                                                |                                         |                           |                | 3.2–7.0                            | 3.2–7.0                            | 3.3–3.8                                  |
| Dissipation (power) factor<br>(60 Hz)                         |                                                                |                                         |                           |                | 0.01–0.06                          | 0.01–0.06                          | 0.01–0.04                                |
| Dissipation factor (10 <sup>6</sup> Hz)                       |                                                                |                                         |                           |                | 0.01–0.06                          | 0.01–0.10                          | 0.01–0.04                                |
| <u>Mechanical</u>                                             |                                                                |                                         |                           |                |                                    |                                    |                                          |
| Compressive modulus,<br>10 <sup>3</sup> lb · in <sup>-2</sup> |                                                                | 300                                     |                           |                |                                    |                                    |                                          |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                             | Alloy                                               | Allyl                            |                           |                | Cellulosic        |           |                                  |
|----------------------------------------------------------------------------------------|-----------------------------------------------------|----------------------------------|---------------------------|----------------|-------------------|-----------|----------------------------------|
|                                                                                        | Polycarbonate acrylonitrile-butadiene-styrene alloy | Allyl-diglycol-carbonate polymer | Diallyl phthalate molding |                | Cellulose acetate |           | Cellulose-acetate-butyrate resin |
|                                                                                        |                                                     |                                  | Glass-filled              | Mineral-filled | Sheet             | Molding   | Sheet                            |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$      | 11                                                  | 21–23                            | 25–35                     | 20–32          | 22–33             | 25–36     |                                  |
| Elongation at break, %                                                                 | 10–15                                               |                                  | 3–5                       | 3–5            | 17–40             | 6–40      | 50–100                           |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                       | 300–400                                             | 250–330                          | 1200–1500                 | 1000–1400      |                   |           | 740–1300                         |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$            | 13.0–13.7                                           | 6–13                             | 9–20                      | 8.5–11         | 6–10              | 2–16      | 4–9                              |
| Hardness, Rockwell (or Shore)                                                          | R117                                                | M95–M100                         | E80–E87                   | E61            | R85–R120          | R100–R123 | R50–R95                          |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                         | 560                                                 | 11–21                            | 21–800                    | 16–43          | 107–454           | 53–214    | 133–288                          |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                | 370–380                                             | 300                              | 1400–2200                 | 1200–2200      |                   |           | 200–250                          |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                      | 7.0–7.3                                             | 5–6                              | 6–11                      | 5–8            | 4.5–8.0           | 1.9–9.0   | 2.6–6.9                          |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 8.5                                                 |                                  |                           |                | 2.2–7.4           | 4.1–7.6   |                                  |
| <b>Thermal</b>                                                                         |                                                     |                                  |                           |                |                   |           |                                  |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                        |                                                     |                                  |                           |                |                   | 1.3–3.8   | 1.3–3.8                          |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                      | 63–67                                               | 5.4–9.6                          | 0.68–2.4                  | 2.8            | 100–150           | 80–180    | 110–170                          |
| Deflection temperature under flexural load (264 $\text{lb} \cdot \text{in}^{-2}$ ), °C | 104–116                                             | 60–88                            | 165–288+                  | 160–288        | 44–91             | 51–98     | 49–58                            |
| Maximum recommended service temperature, °C                                            |                                                     |                                  |                           |                |                   |           |                                  |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                        |                                                     |                                  |                           |                | 0.3–0.4           | 0.3–0.42  | 0.3–0.4                          |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$               | 0.25–0.38                                           | 0.20–0.21                        | 0.21–0.63                 | 0.30–1.04      | 0.17–0.34         | 0.17–0.34 | 0.17–0.34                        |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Cellulosic                                |                                             |                 |                   | Chlorinated polyether | Epoxy                  |                |
|------------------------------------------------------------|-------------------------------------------|---------------------------------------------|-----------------|-------------------|-----------------------|------------------------|----------------|
|                                                            | Cellulose-acetate butyrate resin, molding | Cellulose-acetate propionate resin, molding | Ethyl cellulose | Cellulose nitrate |                       | Bisphenol              |                |
|                                                            |                                           |                                             |                 |                   |                       | Glass-fiber-reinforced | Mineral-filled |
| <u>Physical</u>                                            |                                           |                                             |                 |                   |                       |                        |                |
| Melting temperature, °C                                    |                                           |                                             |                 |                   |                       |                        |                |
| Crystalline                                                | 140                                       | 190                                         | 135             |                   | 125                   | Thermoset              | Thermoset      |
| Amorphous                                                  |                                           |                                             |                 |                   |                       |                        |                |
| Specific gravity                                           | 1.15–1.22                                 | 1.17–1.24                                   | 1.09–1.17       | 1.35–1.40         | 1.4                   | 1.6–2.0                | 1.6–2.1        |
| Water absorption (24 h), %                                 | 0.9–2.2                                   | 1.2–2.8                                     | 0.8–1.8         |                   |                       | 0.04–0.20              | 0.03–0.20      |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 9–13                                      | 12–17.7                                     | 13.8–19.7       |                   |                       | 9.8–15.7               | 9.8–15.7       |
| <u>Electrical</u>                                          |                                           |                                             |                 |                   |                       |                        |                |
| Volume (dc) resistivity, ohm-cm                            | 10 <sup>10</sup> –10 <sup>12</sup>        |                                             |                 | 10 <sup>10</sup>  |                       |                        |                |
| Dielectric constant (60 Hz)                                | 3.5–6.4                                   |                                             |                 | 7.0–7.5           |                       |                        |                |
| Dielectric constant (10 <sup>6</sup> Hz)                   | 3.2–6.2                                   |                                             | 3.01            | 6.6               |                       |                        |                |
| Dissipation (power) factor (60 Hz)                         | 0.01–0.04                                 |                                             |                 |                   |                       |                        |                |
| Dissipation factor (10 <sup>6</sup> Hz)                    | 0.01–0.04                                 |                                             |                 |                   |                       |                        |                |
| <u>Mechanical</u>                                          |                                           |                                             |                 |                   |                       |                        |                |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> |                                           |                                             |                 |                   |                       | 3000                   |                |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Cellulosic                                |                                             |                 |                   | Chlorinated polyether | Epoxy                  |                |
|------------------------------------------------------------------------------------------|-------------------------------------------|---------------------------------------------|-----------------|-------------------|-----------------------|------------------------|----------------|
|                                                                                          | Cellulose-acetate butyrate resin, molding | Cellulose-acetate propionate resin, molding | Ethyl cellulose | Cellulose nitrate |                       | Bisphenol              |                |
|                                                                                          |                                           |                                             |                 |                   |                       | Glass-fiber-reinforced | Mineral-filled |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 2.1–7.5                                   | 2.4–7.0                                     | 5–40            | 2.1–8.0           | 600–800               | 18,000–40,000          | 18,000–40,000  |
| Elongation at break, %                                                                   | 40–88                                     | 29–100                                      |                 | 40–45             |                       | 4                      |                |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 90–300                                    | 120–350                                     |                 |                   |                       | 2–4.5                  |                |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              | 1.8–9.3                                   | 2.9–11.4                                    | 4–12            | 9–11              | 5                     | 8–30                   | 6–18           |
| Hardness, Rockwell (or Shore)                                                            | R31–R116                                  | R10–R122                                    | R50–R115        | R95–R115          | R100                  | M100–M112              | M100–M112      |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | 53–582                                    | 27 to no break                              | 21              | 267–374           | 21                    | 16–533                 | 16–22          |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  | 50–200                                    | 60–215                                      |                 | 190–220           |                       | 3                      |                |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 2.6–6.9                                   | 2.0–7.8                                     | 2–8             | 7–8               | 1.5–1.8               | 5–20                   | 4–10           |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                                           |                                             |                 |                   |                       |                        |                |
| Thermal                                                                                  |                                           |                                             |                 |                   |                       |                        |                |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          | 1.3–3.8                                   |                                             |                 |                   | Self-extinguishing    |                        |                |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                        | 110–170                                   | 110–170                                     | 100–200         | 80–120            | 6.6                   | 11–50                  | 20–60          |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C | 44–94                                     | 44–109                                      | 45–88           | 60–71             | 185                   | 107–260                | 107–260        |
| Maximum recommended service temperature, °C                                              |                                           |                                             |                 |                   | 255                   |                        |                |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          | 0.3–0.4                                   |                                             |                 | 0.31–0.41         |                       |                        |                |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.17–0.30                                 | 0.17–0.30                                   | 0.16–0.30       | 0.23              |                       | 0.17–0.42              | 0.17–1.48      |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                    | Epoxy                              |           |                | Fluorocarbon              |                            |                                         |                 |
|---------------------------------------------------------------|------------------------------------|-----------|----------------|---------------------------|----------------------------|-----------------------------------------|-----------------|
|                                                               | Casting resin                      |           | Novolac resin  | Poly(tetrafluoroethylene) |                            | Poly(chloro-<br>trifluoro-<br>ethylene) | Perfluoroalkoxy |
|                                                               | Unfilled                           | Flexible  | Mineral-filled | Granular                  | Glass-fiber-<br>reinforced |                                         |                 |
| <u>Physical</u>                                               |                                    |           |                |                           |                            |                                         |                 |
| Melting temperature, °C                                       |                                    |           |                |                           |                            |                                         |                 |
| Crystalline                                                   | Thermoset                          | Thermoset | Thermoset      | 327                       | 327                        | 220                                     | 310             |
| Amorphous                                                     |                                    |           |                |                           |                            |                                         |                 |
| Specific gravity                                              | 1.11–1.40                          | 1.05–1.35 | 1.7–2.1        | 2.14–2.20                 | 2.2–2.3                    | 2.1–2.2                                 | 2.12–2.17       |
| Water absorption (24 h), %                                    | 0.08–0.15                          | 0.27–0.50 | 0.05–0.2       | 0.01                      |                            | 0.03                                    |                 |
| Dielectric strength,<br>kV · mm <sup>−1</sup>                 | 11.8–19.7                          | 9.3–15.8  | 11.8–13.8      | 18.9                      | 12.6                       | 19.7–23                                 | 19.7            |
| <u>Electrical</u>                                             |                                    |           |                |                           |                            |                                         |                 |
| Volume (dc) resistivity,<br>ohm-cm                            | 10 <sup>12</sup> –10 <sup>17</sup> |           |                | 10 <sup>18</sup>          |                            | 10 <sup>18</sup>                        |                 |
| Dielectric constant (60 Hz)                                   | 3.5–5.0                            |           |                | 2.1                       |                            | 2.3–2.7                                 |                 |
| Dielectric constant (10 <sup>6</sup> Hz)                      | 3.5–5.0                            |           |                | 2.1                       |                            | 2.3–2.5                                 |                 |
| Dissipation (power) factor (60<br>Hz)                         |                                    |           |                | 0.0002                    |                            | 0.001                                   |                 |
| Dissipation factor (10 <sup>6</sup> Hz)                       |                                    |           |                | 0.0002                    |                            | 0.005                                   |                 |
| <u>Mechanical</u>                                             |                                    |           |                |                           |                            |                                         |                 |
| Compressive modulus,<br>10 <sup>3</sup> lb · in <sup>−2</sup> |                                    |           |                | 60                        |                            |                                         |                 |



**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                                   | Epoxy         |          |                | Fluorocarbon                                 |                            |                                              |                                             |
|--------------------------------------------------------------------------------------------------------------|---------------|----------|----------------|----------------------------------------------|----------------------------|----------------------------------------------|---------------------------------------------|
|                                                                                                              | Casting resin |          | Novolac resin  | Poly(tetrafluoroethylene)                    |                            | Poly(chloro-<br>trifluoro-<br>ethylene)      | Perfluoroalkoxy                             |
|                                                                                                              | Unfilled      | Flexible | Mineral-filled | Granular                                     | Glass-fiber-<br>reinforced |                                              |                                             |
| Compressive strength, rupture<br>or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 15–25         | 1–14     | 30             | 1.7                                          |                            | 4.6–7.4                                      |                                             |
| Elongation at break, %                                                                                       | 3–6           | 20–70    | 2–4            | 200–400                                      | 200–300                    | 80–250                                       | 300                                         |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                                          |               |          | 2000           | 80                                           | 235                        | 120                                          |                                             |
| Flexural strength, rupture or<br>yield, $10^{-3} \text{ lb} \cdot \text{in}^{-2}$                            | 13–21         | 1–13     | 16–20          |                                              | 2                          | 7.4–9.3                                      |                                             |
| Hardness, Rockwell (or Shore)                                                                                | M80–M110      |          |                | (D50–D55)                                    | (D60–D70)                  | R75–R95                                      | (D64)                                       |
| Impact strength (Izod) at<br>23°C, $\text{J} \cdot \text{m}^{-1}$                                            | 10.7–53       | 187–267  | 21             | 160                                          | 144                        | 133–160                                      | No break                                    |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                                      | 350           | 1–350    |                | 58–80                                        |                            | 150–300                                      |                                             |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                                         | 4–13          | 2–10     | 6–12           | 2–5                                          | 2–2.7                      | 4.5–6                                        | 4–4.3                                       |
| Tensile yield strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                                            |               |          | 30             |                                              |                            |                                              |                                             |
| <u>Thermal</u>                                                                                               |               |          |                |                                              |                            |                                              |                                             |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                                              |               |          |                | Self-<br>extinguishing                       | Self-<br>extinguishing     | Self-<br>extinguishing                       |                                             |
| Coefficient of linear thermal<br>expansion, $10^{-6}^\circ\text{C}$                                          | 45–65         | 20–100   | 22–30          | 100                                          | 77–100                     | 70                                           |                                             |
| Deflection temperature under<br>flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ),<br>$^\circ\text{C}$ | 46–288        | 23–121   | 149–260        | 121 ( $66 \text{ lb} \cdot \text{in}^{-2}$ ) |                            | 126 ( $66 \text{ lb} \cdot \text{in}^{-2}$ ) | 74 ( $66 \text{ lb} \cdot \text{in}^{-2}$ ) |
| Maximum recommended<br>service temperature, $^\circ\text{C}$                                                 |               |          |                | 260                                          |                            | 200                                          |                                             |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                                              |               |          |                | 0.25                                         |                            | 0.22                                         |                                             |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                                  | 0.17–0.21     |          |                | 0.25                                         | 0.34–0.40                  | 0.19–0.22                                    | 0.25                                        |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Fluorocarbon                         |                           |                                        |                        |                                            | Melamine formaldehyde |                        |
|------------------------------------------------------------|--------------------------------------|---------------------------|----------------------------------------|------------------------|--------------------------------------------|-----------------------|------------------------|
|                                                            | Fluorinated ethylene-propylene resin | Poly(vinylidene fluoride) | Ethylene-tetrafluoroethylene copolymer |                        | Ethylene-chlorotrifluoroethylene copolymer | Cellulose-filled      | Glass-fiber-reinforced |
|                                                            |                                      |                           | Unfilled                               | Glass-fiber-reinforced |                                            |                       |                        |
| <u>Physical</u>                                            |                                      |                           |                                        |                        |                                            |                       |                        |
| Melting temperature, °C                                    |                                      |                           |                                        |                        |                                            |                       |                        |
| Crystalline                                                | 275                                  | 156                       | 270                                    | 270                    | 245                                        | Thermoset             | Thermoset              |
| Amorphous                                                  |                                      |                           |                                        |                        |                                            |                       |                        |
| Specific gravity                                           | 2.14–2.17                            | 1.75–1.78                 | 1.7                                    | 1.8                    | 1.68                                       | 1.47–1.52             | 1.5–2.0                |
| Water absorption (24 h), %                                 | <0.01                                | 0.04–0.06                 | 0.03                                   | 0.02                   | 0.01                                       | 0.1–0.8               | 0.09–1.3               |
| Dielectric strength, kV · mm <sup>-1</sup>                 | 20–24                                | 10                        | 16                                     | 17                     | 19                                         | 11–16                 | 5–15                   |
| <u>Electrical</u>                                          |                                      |                           |                                        |                        |                                            |                       |                        |
| Volume (dc) resistivity, ohm-cm                            |                                      |                           |                                        |                        |                                            |                       |                        |
| Dielectric constant (60 Hz)                                | 2.1                                  | 8–9                       | 2.6                                    |                        | 2.6                                        |                       |                        |
| Dielectric constant (10 <sup>6</sup> Hz)                   | 2.1                                  | 8–9                       | 2.6                                    |                        | 2.6                                        |                       |                        |
| Dissipation (power) factor (60 Hz)                         |                                      | High                      |                                        |                        |                                            |                       |                        |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                                      | High                      |                                        |                        |                                            |                       |                        |
| <u>Mechanical</u>                                          |                                      |                           |                                        |                        |                                            |                       |                        |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>-2</sup> |                                      | 120                       | 120                                    | 1200                   | 240                                        |                       |                        |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Fluorocarbon                                |                           |                                        |                        |                                             | Melamine formaldehyde |                        |
|------------------------------------------------------------------------------------------|---------------------------------------------|---------------------------|----------------------------------------|------------------------|---------------------------------------------|-----------------------|------------------------|
|                                                                                          | Fluorinated ethylene-propylene resin        | Poly(vinylidene fluoride) | Ethylene-tetrafluoroethylene copolymer |                        | Ethylene-chlorotrifluoro-ethylene copolymer | Cellulose-filled      | Glass-fiber-reinforced |
|                                                                                          |                                             |                           | Unfilled                               | Glass-fiber-reinforced |                                             |                       |                        |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 2.2                                         | 8.7–10                    | 7.1                                    | 10                     |                                             | 33–45                 | 20–35                  |
| Elongation at break, %                                                                   | 250–330                                     | 25–500                    | 100–400                                | 8                      | 200–300                                     | 0.6–1.0               | 0.6                    |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 80–95                                       | 200                       | 200                                    | 950                    | 240                                         | 1100                  |                        |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              |                                             | 8.6–11                    | 5.5                                    | 10.7                   | 7                                           | 9–16                  | 14–23                  |
| Hardness, Rockwell (or Shore)                                                            | (D60–D65)                                   | (D80)                     | R50 (D75)                              | R74                    | R95                                         | M115–M125             | M115                   |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | No break                                    | 192–214                   | No break                               | 480                    | No break                                    | 11–21                 | 32–961                 |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  | 50                                          | 120                       | 120                                    | 1200                   | 240                                         | 1.1–1.4               | 1.6–2.4                |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 2.7–3.1                                     | 5.5–7.4                   | 6.5                                    | 12                     | 7                                           | 5–13                  | 5–10.5                 |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                                             |                           |                                        |                        |                                             |                       |                        |
| Thermal                                                                                  |                                             |                           |                                        |                        |                                             |                       |                        |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          | Not combustible                             | Not combustible           | Not combustible                        | Not combustible        | Not combustible                             | Self-extinguishing    | Self-extinguishing     |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                        | 83–105                                      | 85                        | 59                                     | 10–32                  | 80                                          | 40–45                 | 15–28                  |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C | 70 ( $66 \text{ lb} \cdot \text{in}^{-2}$ ) | 80–90                     | 71                                     | 210                    | 77                                          | 177–199               | 190–204                |
| Maximum recommended service temperature, °C                                              | 205                                         | 150                       |                                        |                        |                                             | 210                   |                        |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          | 0.28                                        |                           |                                        |                        |                                             |                       |                        |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.25                                        | 0.19–0.24                 | 0.24                                   |                        | 0.16                                        | 0.27–0.41             | 0.41–0.49              |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Melamine phenolic, woodflour- and cellulose-filled | Nitrile                | Phenolic                                        |                  |                        |                  |                |
|------------------------------------------------------------|----------------------------------------------------|------------------------|-------------------------------------------------|------------------|------------------------|------------------|----------------|
|                                                            |                                                    |                        | Unfilled                                        | Woodflour-filled | Glass-fiber-reinforced | Cellulose-filled | Mineral-filled |
| <u>Physical</u>                                            |                                                    |                        |                                                 |                  |                        |                  |                |
| Melting temperature, °C                                    |                                                    |                        |                                                 |                  |                        |                  |                |
| Crystalline                                                | Thermoset                                          |                        | Thermoset                                       | Thermoset        | Thermoset              | Thermoset        | Thermoset      |
| Amorphous                                                  |                                                    | 95                     |                                                 |                  |                        |                  |                |
| Specific gravity                                           | 1.5–1.7                                            | 1.15                   | 1.24–1.32                                       | 1.37–1.46        | 1.69–2.0               | 1.38–1.42        | 1.42–1.84      |
| Water absorption (24 h), %                                 | 0.3–0.65                                           | 0.28                   | 0.1–0.36                                        | 0.3–1.2          | 0.03–1.2               | 0.5–0.9          | 0.1–0.3        |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 8.7–12.8                                           | 8.7–9.5                | 9.8–15.8                                        | 10.2–15.8        | 5.5–15.8               | 11.8–15          | 7.9–13.8       |
| <u>Electrical</u>                                          |                                                    |                        |                                                 |                  |                        |                  |                |
| Volume (dc) resistivity, ohm-cm                            |                                                    | 1.9 × 10 <sup>15</sup> | 1 × 10 <sup>12</sup><br>to 7 × 10 <sup>12</sup> |                  |                        |                  |                |
| Dielectric constant (60 Hz)                                |                                                    |                        | 6.5–7.5                                         |                  |                        |                  |                |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                                                    |                        | 4.0–5.5                                         |                  |                        |                  |                |
| Dissipation (power) factor (60 Hz)                         |                                                    |                        | 0.10–0.15                                       |                  |                        |                  |                |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                                                    |                        | 0.04–0.05                                       |                  |                        |                  |                |
| <u>Mechanical</u>                                          |                                                    |                        |                                                 |                  |                        |                  |                |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> |                                                    |                        |                                                 |                  |                        |                  |                |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                   | Melamine<br>phenolic,<br>woodflour- and<br>cellulose-<br>filled | Nitrile | Phenolic               |                      |                            |                      |                    |
|----------------------------------------------------------------------------------------------|-----------------------------------------------------------------|---------|------------------------|----------------------|----------------------------|----------------------|--------------------|
|                                                                                              |                                                                 |         | Unfilled               | Woodflour-<br>filled | Glass-fiber-<br>reinforced | Cellulose-<br>filled | Mineral-<br>filled |
| Compressive strength, rupture<br>or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$         | 26–30                                                           | 12      | 18–32                  | 25–31                | 26–70                      | 22–31                | 22.5–34.6          |
| Elongation at break, %                                                                       | 0.4–0.8                                                         | 3–4     | 1.5–2.0                | 0.4–0.8              | 0.2                        | 1–2                  | 0.1–0.5            |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                          | 1000–2000                                                       | 500–590 | 700–1500               | 1000–1200            | 2000–33,000                | 900–1300             | 1000–2000          |
| Flexural strength, rupture or<br>yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$               | 8–10                                                            | 14      | 11–17                  | 7–14                 | 15–60                      | 5.5–11               | 11–14              |
| Hardness, Rockwell (or Shore)                                                                | E95–E100                                                        | M72–M76 | M93–M120               | M100–M115            | E54–E101                   | M95–115              | E88                |
| Impact strength (Izod) at<br>23°C, $\text{J} \cdot \text{m}^{-1}$                            | 11–21                                                           | 80–256  | 13–21                  | 11–32                | 27–960                     | 21–59                | 14–19              |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                      | 800–1700                                                        | 510–580 | 700–1500               | 800–1700             | 1900–3300                  |                      | 2400               |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 6–8                                                             | 9       | 6–9                    | 5–9                  | 7–18                       | 3.5–6.5              | 6–9.7              |
| Tensile yield strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                            |                                                                 |         | 12–15                  |                      |                            |                      |                    |
| <u>Thermal</u>                                                                               |                                                                 |         |                        |                      |                            |                      |                    |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                              |                                                                 |         | Self-<br>extinguishing |                      |                            |                      |                    |
| Coefficient of linear thermal<br>expansion, $10^{-6}^\circ\text{C}$                          | 10–40                                                           | 66      | 68                     | 30–45                | 8–21                       | 20–31                | 19–26              |
| Deflection temperature<br>under flexural load<br>(264 $\text{lb} \cdot \text{in}^{-2}$ ), °C | 140–154                                                         | 73      | 74–80                  | 149–188              | 177–316                    | 149–177              | 320–246            |
| Maximum recommended<br>service temperature, °C                                               |                                                                 |         |                        |                      |                            |                      |                    |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                              |                                                                 |         |                        |                      |                            |                      |                    |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                  | 0.17–0.30                                                       | 0.26    | 0.15                   | 0.17–0.34            | 0.34–0.59                  | 0.25–0.38            | 0.42–0.57          |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                    | Polyamide                |                                      |                          |                                    |                                    |                                    |                                    |
|---------------------------------------------------------------|--------------------------|--------------------------------------|--------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|
|                                                               | Nylon 6                  |                                      |                          |                                    | Nylon 6/6                          |                                    | Nylon 6/6-<br>nylon 6<br>copolymer |
|                                                               | Molding and<br>extrusion | 30–35%<br>glass-fiber-<br>reinforced | High-impact<br>copolymer | Molding                            | 33% glass-<br>fiber-<br>reinforced | Molybdenum<br>disulfide-<br>filled |                                    |
| <u>Physical</u>                                               |                          |                                      |                          |                                    |                                    |                                    |                                    |
| Melting temperature, °C                                       |                          |                                      |                          |                                    |                                    |                                    |                                    |
| Crystalline                                                   | 216                      | 216                                  | 216                      | 265                                | 265                                | 265                                | 240                                |
| Amorphous                                                     |                          |                                      |                          |                                    |                                    |                                    |                                    |
| Specific gravity                                              | 1.12–1.14                | 1.35–1.42                            | 1.08–1.17                | 1.13–1.15                          | 1.38                               | 1.15–1.17                          | 1.08–1.14                          |
| Water absorption (24 h), %                                    | 2.9                      | 1.2                                  | 1.3–1.5                  | 1.0–1.3                            | 1.0                                | 0.8–1.1                            | 1.5–2.0                            |
| Dielectric strength, kV · mm <sup>−1</sup>                    | 15.8                     | 15.8                                 | 22                       | 24                                 |                                    | 14                                 | 15.8                               |
| <u>Electrical</u>                                             |                          |                                      |                          |                                    |                                    |                                    |                                    |
| Volume (dc) resistivity,<br>ohm-cm                            | 10 <sup>12</sup>         |                                      |                          | 10 <sup>12</sup> –10 <sup>15</sup> |                                    |                                    | 10 <sup>10</sup>                   |
| Dielectric constant (60 Hz)                                   | 9.8                      |                                      |                          | 4.0                                |                                    |                                    | 16                                 |
| Dielectric constant (10 <sup>6</sup> Hz)                      | 3.7                      |                                      |                          | 3.6                                |                                    |                                    | 4                                  |
| Dissipation (power) factor<br>(60 Hz)                         | 0.14                     |                                      |                          | 0.01–0.02                          |                                    |                                    | 0.4                                |
| Dissipation factor (10 <sup>6</sup> Hz)                       | 0.12                     |                                      |                          | 0.02–0.03                          |                                    |                                    | 0.1                                |
| <u>Mechanical</u>                                             |                          |                                      |                          |                                    |                                    |                                    |                                    |
| Compressive modulus,<br>10 <sup>3</sup> lb · in <sup>−2</sup> | 250                      |                                      |                          |                                    |                                    |                                    |                                    |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                     | Polyamide                |                                      |                          |                        |                                    |                                    |                                    |
|------------------------------------------------------------------------------------------------|--------------------------|--------------------------------------|--------------------------|------------------------|------------------------------------|------------------------------------|------------------------------------|
|                                                                                                | Nylon 6                  |                                      |                          |                        | Nylon 6/6                          |                                    | Nylon 6/6-<br>nylon 6<br>copolymer |
|                                                                                                | Molding and<br>extrusion | 30–35%<br>glass-fiber-<br>reinforced | High-impact<br>copolymer | Molding                | 33% glass-<br>fiber-<br>reinforced | Molybdenum<br>disulfide-<br>filled |                                    |
| Compressive strength, rupture<br>or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$           | 13–16                    | 19                                   |                          | 15 (yield)             | 24.9                               | 12.5                               |                                    |
| Elongation at break, %                                                                         | 30–100                   | 3–6                                  | 150–270                  | 60                     | 3                                  | 15                                 | 40                                 |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                            | 390                      | 1500                                 | 110–320                  | 420                    | 1300                               | 450                                | 150–410                            |
| Flexural strength, rupture or<br>yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$                 | 14                       | 33                                   | 5–12                     | 17                     | 41                                 | 17                                 |                                    |
| Hardness, Rockwell (or Shore)                                                                  | R119                     | M101                                 | R81–R110                 | R120                   | M100                               | R119                               | R119                               |
| Impact strength (Izod) at<br>23°C, $\text{J} \cdot \text{m}^{-1}$                              | 32–53                    | 160                                  | 96 to no<br>break        | 43–53                  | 117                                | 240                                | 37                                 |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                        | 380                      | 1450                                 |                          |                        |                                    | 550                                | 150–410                            |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                           | 11.8                     | 25                                   | 7.5–11                   | 12                     | 28                                 | 13.7                               | 7.4–12.4                           |
| Tensile yield strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                              | 8                        |                                      |                          | 8                      |                                    |                                    |                                    |
| Thermal                                                                                        |                          |                                      |                          |                        |                                    |                                    |                                    |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                                | Self-<br>extinguishing   | Self-<br>extinguishing               | Self-<br>extinguishing   | Self-<br>extinguishing | Self-<br>extinguishing             | Self-<br>extinguishing             | Self-<br>extinguishing             |
| Coefficient of linear thermal<br>expansion, $10^{-6}/^\circ\text{C}$                           | 80–90                    | 20–30                                | 30–40                    | 80                     | 15–20                              | 54                                 |                                    |
| Deflection temperature under<br>flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ),<br>°C | 68–85                    | 210                                  | 45–54                    | 75                     | 249                                | 127                                | 77                                 |
| Maximum recommended<br>service temperature, °C                                                 | 107                      |                                      |                          | 135                    |                                    |                                    |                                    |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                                | 0.4                      |                                      |                          | 0.4                    |                                    |                                    |                                    |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                    | 0.24                     | 0.24                                 |                          | 0.24                   | 0.22                               |                                    |                                    |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Polyamide                        |                  |                               |                                 |                                 |                                              | Poly(amide-imide), unfilled |
|------------------------------------------------------------|----------------------------------|------------------|-------------------------------|---------------------------------|---------------------------------|----------------------------------------------|-----------------------------|
|                                                            | Nylon 6/9, molding and extrusion | Nylon 6/12       |                               | Nylon 11, molding and extrusion | Nylon 12, molding and extrusion | Aromatic nylon (aramid), molded and unfilled |                             |
|                                                            |                                  | Molding          | 30–35% glass-fiber-reinforced |                                 |                                 |                                              |                             |
| <u>Physical</u>                                            |                                  |                  |                               |                                 |                                 |                                              |                             |
| Melting temperature, °C                                    |                                  |                  |                               |                                 |                                 |                                              |                             |
| Crystalline                                                | 205                              | 217              | 217                           | 194                             | 179                             | 275                                          | 275                         |
| Amorphous                                                  |                                  |                  |                               |                                 |                                 |                                              |                             |
| Specific gravity                                           | 1.08–1.10                        | 1.06–1.08        | 1.31–1.38                     | 1.03–1.05                       | 1.01–1.02                       | 1.30                                         | 1.40                        |
| Water absorption (24 h), %                                 | 0.5                              | 0.4              | 0.2                           | 0.3                             | 0.25                            | 0.6                                          | 0.28                        |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 24                               | 16               | 21                            | 17                              | 18                              | 31                                           | 24                          |
| <u>Electrical</u>                                          |                                  |                  |                               |                                 |                                 |                                              |                             |
| Volume (dc) resistivity, ohm-cm                            |                                  | 10 <sup>15</sup> |                               |                                 | 10 <sup>14</sup>                |                                              |                             |
| Dielectric constant (60 Hz)                                |                                  | 4.0              |                               |                                 | 3.8                             |                                              |                             |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                                  | 3.5              |                               |                                 | 3.0                             |                                              |                             |
| Dissipation (power) factor (60 Hz)                         |                                  | 0.02             |                               |                                 | 0.07                            |                                              |                             |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                                  | 0.02             |                               |                                 | 0.04                            |                                              |                             |
| <u>Mechanical</u>                                          |                                  |                  |                               |                                 |                                 |                                              |                             |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> |                                  |                  |                               | 180                             |                                 | 290                                          | 413                         |



**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Polyamide                        |            |                               |                                 |                                 |                                              | Poly(amide-imide), unfilled |
|------------------------------------------------------------------------------------------|----------------------------------|------------|-------------------------------|---------------------------------|---------------------------------|----------------------------------------------|-----------------------------|
|                                                                                          | Nylon 6/9, molding and extrusion | Nylon 6/12 |                               | Nylon 11, molding and extrusion | Nylon 12, molding and extrusion | Aromatic nylon (aramid), molded and unfilled |                             |
|                                                                                          |                                  | Molding    | 30–35% glass-fiber-reinforced |                                 |                                 |                                              |                             |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 1125                             | 2.4        | 4                             | 300                             | 7.5                             | 30                                           | 40                          |
| Elongation at break, %                                                                   |                                  | 150        |                               |                                 | 300                             | 5                                            | 12–18                       |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 290                              | 290        | 1120                          | 150                             | 165                             | 640                                          | 664                         |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              | R111                             | R114       | E40–E50                       | R108                            | 1.5                             | 25.8                                         | 30                          |
| Hardness, Rockwell (or Shore)                                                            |                                  |            |                               |                                 | R106–R109                       | E90                                          | E78                         |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | 59                               | 53         | 139                           | 96                              | 107–300                         | 75                                           | 133                         |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  | 275                              | 290        | 1200                          | 185                             | 180                             |                                              | 730                         |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 8.5                              | 8.8        | 24                            | 8                               | 8–9                             | 17.5                                         | 26.9                        |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                                  | 8.8        |                               |                                 |                                 |                                              |                             |
| <u>Thermal</u>                                                                           |                                  |            |                               |                                 |                                 |                                              |                             |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          |                                  |            |                               | Self-extinguishing              |                                 |                                              |                             |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                        |                                  | 90         |                               | 55–100                          | 67–100                          | 40                                           | 36                          |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C | 57–60                            | 82         | 93–218                        | 54                              | 54                              | 260                                          | 274                         |
| Maximum recommended service temperature, °C                                              |                                  |            |                               | 100–120                         |                                 |                                              | 260                         |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          |                                  | 0.4        |                               | 0.58                            |                                 |                                              |                             |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 |                                  | 0.22       |                               | 0.34                            | 0.22                            | 0.22                                         | 0.25                        |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                    | Poly(aryl<br>ether),<br>unfilled | Polycarbonate        |                                   | Thermoplastic polyester      |                                |                              |                                |
|---------------------------------------------------------------|----------------------------------|----------------------|-----------------------------------|------------------------------|--------------------------------|------------------------------|--------------------------------|
|                                                               |                                  | Low<br>viscosity     | 30% glass-<br>fiber<br>reinforced | Poly(butylene terephthalate) |                                | Poly(ethylene terephthalate) |                                |
|                                                               |                                  |                      |                                   | Unfilled                     | 30% glass-fiber-<br>reinforced | Unfilled                     | 30% glass-fiber-<br>reinforced |
| <u>Physical</u>                                               |                                  |                      |                                   |                              |                                |                              |                                |
| Melting temperature, °C                                       |                                  |                      |                                   |                              |                                |                              |                                |
| Crystalline                                                   |                                  |                      |                                   | 232–267                      | 232–267                        | 245                          | 245                            |
| Amorphous                                                     | 160                              | 140                  | 150                               |                              |                                |                              |                                |
| Specific gravity                                              | 1.14                             | 1.2                  | 1.4                               | 1.31–1.38                    | 1.52                           | 1.34–1.39                    | 1.27                           |
| Water absorption (24 h), %                                    | 0.25                             | 0.15                 | 0.14                              | 0.08–0.09                    | 0.06–0.08                      | 0.1–0.2                      | 0.05                           |
| Dielectric strength, kV · mm <sup>−1</sup>                    | 17                               | 15                   | 19                                | 16–22                        | 18–22                          |                              | 22                             |
| <u>Electrical</u>                                             |                                  |                      |                                   |                              |                                |                              |                                |
| Volume (dc) resistivity,<br>ohm-cm                            |                                  | 2 × 10 <sup>16</sup> | > 10 <sup>16</sup>                |                              | 10 <sup>16</sup>               | 10 <sup>16</sup>             |                                |
| Dielectric constant (60 Hz)                                   |                                  | 3.17                 | 3.35                              |                              |                                |                              |                                |
| Dielectric constant (10 <sup>6</sup> Hz)                      |                                  | 2.96                 | 3.31                              |                              |                                | 3.25                         |                                |
| Dissipation (power) factor<br>(60 Hz)                         |                                  | 0.0009               | 0.011                             |                              |                                |                              |                                |
| Dissipation factor (10 <sup>6</sup> Hz)                       |                                  | 0.010                | 0.007                             |                              |                                |                              |                                |
| <u>Mechanical</u>                                             |                                  |                      |                                   |                              |                                |                              |                                |
| Compressive modulus,<br>10 <sup>3</sup> lb · in <sup>−2</sup> |                                  | 350                  | 1300                              |                              |                                |                              |                                |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                     | Poly(aryl<br>ether),<br>unfilled | Polycarbonate          |                                   | Thermoplastic polyester      |                                |                              |                                |
|------------------------------------------------------------------------------------------------|----------------------------------|------------------------|-----------------------------------|------------------------------|--------------------------------|------------------------------|--------------------------------|
|                                                                                                |                                  | Low<br>viscosity       | 30% glass-<br>fiber<br>reinforced | Poly(butylene terephthalate) |                                | Poly(ethylene terephthalate) |                                |
|                                                                                                |                                  |                        |                                   | Unfilled                     | 30% glass-fiber-<br>reinforced | Unfilled                     | 30% glass-fiber-<br>reinforced |
| Compressive strength, rupture<br>or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$           | 80                               | 12.5                   | 18                                | 8.6–14.5                     | 18–23.5                        | 11–15                        | 25                             |
| Elongation at break, %                                                                         |                                  | 110                    | 3–5                               | 50–300                       | 2–4                            | 50–300                       | 3                              |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                            | 300                              | 340                    | 1100                              | 330–400                      | 1100–1200                      | 35–450                       | 1440                           |
| Flexural strength, rupture or<br>yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$                 | 11                               | 13.5                   | 23                                | 12–16.7                      | 26–29                          | 14–18                        | 33.5                           |
| Hardness, Rockwell (or Shore)                                                                  | R117                             | M70                    | M92                               | M68–M78                      | M90                            | M94–M101                     | M100                           |
| Impact strength (Izod) at<br>23°C, $\text{J} \cdot \text{m}^{-1}$                              | 427                              | 14                     | 107                               | 43–53                        | 69–85                          | 13–32                        | 101                            |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                        | 320                              | 345                    | 1250                              | 280                          | 1300                           | 400–600                      | 1440                           |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                           | 7.5                              | 9.5                    | 19                                | 8.2                          | 17–19                          | 8.5–10.5                     | 23                             |
| Tensile yield strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                              |                                  | 9.0                    |                                   |                              |                                |                              |                                |
| <b>Thermal</b>                                                                                 |                                  |                        |                                   |                              |                                |                              |                                |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                                |                                  | Self-<br>extinguishing | Self-<br>extinguishing            |                              |                                |                              |                                |
| Coefficient of linear thermal<br>expansion, $10^{-6}^\circ\text{C}$                            | 65                               | 68                     | 22                                | 60–95                        | 25                             | 65                           | 29                             |
| Deflection temperature under<br>flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ),<br>°C | 149                              | 138–145                | 146                               | 50–85                        | 220                            | 38–41                        | 224                            |
| Maximum recommended<br>service temperature, °C                                                 |                                  | 143                    |                                   |                              |                                |                              |                                |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                                |                                  | 0.3                    |                                   |                              |                                | 0.27                         |                                |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                    | 0.30                             | 0.20                   | 0.22                              | 0.18–0.30                    | 0.30                           | 0.15                         |                                |



**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                     | Thermoplastic polyester   |                      | Thermosetting and alkyd polyester               |                                        |                          |                            | Polyimide,<br>unfilled |
|------------------------------------------------------------------------------------------------|---------------------------|----------------------|-------------------------------------------------|----------------------------------------|--------------------------|----------------------------|------------------------|
|                                                                                                | Aromatic polyester        |                      | Unsaturated polyester                           |                                        | Alkyd molding compounds  |                            |                        |
|                                                                                                | Extrusion-<br>transparent | Injection<br>molding | Styrene-maleic<br>acid copolymer,<br>low-shrink | Butadiene-<br>maleic acid<br>copolymer | Putty,<br>mineral-filled | Glass-fiber-<br>reinforced |                        |
| Compressive strength, rupture<br>or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$           | 225                       | 10                   | 15–30                                           | 14–30                                  | 12–38                    | 15–36                      | 30–40                  |
| Elongation at break, %                                                                         |                           | 7–10                 | 3–5                                             |                                        |                          |                            | 8–10                   |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                            | 290                       | 700                  | 1000–2500                                       |                                        | 2000                     | 2000                       | 450–500                |
| Flexural strength, rupture or<br>yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$                 | 10.6                      | 12                   | 9–35                                            | 16–24                                  | 6–17                     | 8.5–26                     | 19–28.8                |
| Hardness, Rockwell (or Shore)                                                                  | R105                      |                      | 40–70 (Barcol)                                  | 50–60 (Barcol)                         | E98                      | E95                        | E52–E99                |
| Impact strength (Izod) at<br>23°C, $\text{J} \cdot \text{m}^{-1}$                              | 101                       |                      | 133–800                                         | 214–694                                | 16–27                    | 27–854                     | 80                     |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                        |                           | 300                  | 1000–2500                                       | 1500–2500                              | 500–3000                 |                            | 300                    |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                           | 6                         | 11                   | 4.5–20                                          | 5–10                                   | 3–9                      | 4–9.5                      | 10.5–17.1              |
| Tensile yield strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                              | 7                         |                      |                                                 |                                        |                          |                            | 12.5                   |
| Thermal                                                                                        |                           |                      |                                                 |                                        |                          |                            |                        |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                                |                           |                      |                                                 |                                        |                          |                            |                        |
| Coefficient of linear thermal<br>expansion, $10^{-6}/^\circ\text{C}$                           |                           | 29                   | 6–30                                            |                                        | 20–50                    | 15–33                      | 45–56                  |
| Deflection temperature under<br>flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ),<br>°C | 63                        | 282                  | 190–260                                         | 160–177                                | 177–260                  | 204–260                    | 277–360                |
| Maximum recommended<br>service temperature, °C                                                 |                           |                      |                                                 |                                        |                          |                            |                        |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                                |                           |                      |                                                 |                                        |                          |                            | 0.27                   |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                    |                           | 0.29                 |                                                 | 0.76–0.93                              | 0.51–0.89                | 0.6–0.89                   | 0.10–0.11              |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                    | Poly(methyl<br>pentene),<br>unfilled | Polyolefin         |                    |                    |                                     |                                             |                                         |
|---------------------------------------------------------------|--------------------------------------|--------------------|--------------------|--------------------|-------------------------------------|---------------------------------------------|-----------------------------------------|
|                                                               |                                      | Polyethylene       |                    |                    |                                     |                                             |                                         |
|                                                               |                                      | Low-density        | Medium-density     | High-density       | Ultra high-<br>molecular-<br>weight | Glass-fiber-<br>reinforced,<br>high-density | Ethylene-<br>vinyl acetate<br>copolymer |
| <u>Physical</u>                                               |                                      |                    |                    |                    |                                     |                                             |                                         |
| Melting temperature, °C                                       | 230–240                              |                    |                    |                    |                                     |                                             |                                         |
| Crystalline                                                   |                                      |                    |                    |                    |                                     |                                             | 65–90                                   |
| Amorphous                                                     |                                      | 95–130             | 120–140            | 120–140            | 125–135                             | 120–140                                     |                                         |
| Specific gravity                                              | 0.84                                 | 0.910–0.925        | 0.926–0.94         | 0.941–0.965        | 0.94                                | 1.28                                        | 0.92–0.95                               |
| Water absorption (24 h), %                                    | 0.01                                 | <0.01              | <0.01              | <0.01              | <0.01                               | 0.02                                        | 0.05–0.13                               |
| Dielectric strength, kV · mm <sup>−1</sup>                    |                                      | 18–39              | 18–39              | 18–39              | 28                                  | 20                                          | 24–30                                   |
| <u>Electrical</u>                                             |                                      |                    |                    |                    |                                     |                                             |                                         |
| Volume (dc) resistivity,<br>ohm-cm                            |                                      | > 10 <sup>15</sup> | > 10 <sup>15</sup> | < 10 <sup>15</sup> |                                     |                                             |                                         |
| Dielectric constant (60 Hz)                                   |                                      | 2.3                | 2.3                | 2.3                |                                     |                                             |                                         |
| Dielectric constant (10 <sup>6</sup> Hz)                      |                                      | 2.3                | 2.3                | 2.3                |                                     |                                             |                                         |
| Dissipation (power) factor<br>(60 Hz)                         |                                      | <0.0005            | <0.0005            | <0.0005            |                                     |                                             |                                         |
| Dissipation factor (10 <sup>6</sup> Hz)                       |                                      | <0.0005            | <0.0005            | <0.0005            |                                     |                                             |                                         |
| <u>Mechanical</u>                                             |                                      |                    |                    |                    |                                     |                                             |                                         |
| Compressive modulus,<br>10 <sup>3</sup> lb · in <sup>−2</sup> | 114–171                              |                    |                    |                    |                                     |                                             |                                         |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                                     | Poly(methyl<br>pentene),<br>unfilled | Polyolefin   |                |              |                                     |                                             |                                         |
|------------------------------------------------------------------------------------------------|--------------------------------------|--------------|----------------|--------------|-------------------------------------|---------------------------------------------|-----------------------------------------|
|                                                                                                |                                      | Polyethylene |                |              |                                     |                                             |                                         |
|                                                                                                |                                      | Low-density  | Medium-density | High-density | Ultra high-<br>molecular-<br>weight | Glass-fiber-<br>reinforced,<br>high-density | Ethylene-<br>vinyl acetate<br>copolymer |
| Compressive strength, rupture<br>or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$           | 5–6.6                                |              |                | 2.7–3.6      |                                     | 7                                           |                                         |
| Elongation at break, %                                                                         | 10–50                                | 90–800       | 50–600         | 20–130       | 450–525                             | 1.5                                         | 550–900                                 |
| Flexural modulus at 23°C,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                            | 110–260                              | 8–60         | 60–115         | 100–260      | 130–140                             | 800                                         | 1–20                                    |
| Flexural strength, rupture or<br>yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$                 | 4–6.5                                |              |                |              |                                     | 11                                          |                                         |
| Hardness, Rockwell (or Shore)                                                                  | L67–L74                              | (D40–D51)    | (D50–D60)      | R30–R50      | R50                                 | R75                                         |                                         |
| Impact strength (Izod) at<br>23°C, $\text{J} \cdot \text{m}^{-1}$                              | 16–64                                | No break     | 27–854         | 27–1068      | No break                            | 59                                          | No break                                |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                        | 160–280                              | 14–38        | 25–55          | 60–180       |                                     |                                             | 20–120                                  |
| Tensile strength at break,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                           | 3.5–4                                | 0.6–2.3      | 1.2–3.5        | 3.1–5.5      | 5.6                                 | 9                                           | 1.4–2.8                                 |
| Tensile yield, strength,<br>$10^3 \text{ lb} \cdot \text{in}^{-2}$                             |                                      | 0.8–1.2      | 1.0–2.2        | 3–4          | 3.1–4.0                             |                                             |                                         |
| Thermal                                                                                        |                                      |              |                |              |                                     |                                             |                                         |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                                |                                      | 1.0          | 1.0            | 1.0          |                                     |                                             |                                         |
| Coefficient of linear thermal<br>expansion, $10^{-6}/^\circ\text{C}$                           | 117                                  | 100–200      | 140–160        | 110–130      | 130                                 | 48                                          | 160–200                                 |
| Deflection temperature under<br>flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ),<br>°C | 41                                   | 32–41        | 41–49          | 43–54        | 43–49                               | 121                                         | 34                                      |
| Maximum recommended<br>service temperature, °C                                                 | 175                                  | 70           | 93             | 200          |                                     |                                             |                                         |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                                |                                      | 0.55         | 0.55           | 0.46–0.55    |                                     |                                             |                                         |
| Thermal conductivity,<br>$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                    | 0.17                                 | 0.34         | 0.34–0.42      | 0.46–0.51    |                                     | 0.46                                        |                                         |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Polyolefin             |                  |                  |                  |             | Poly(phenylene sulfide) |                            |
|------------------------------------------------------------|------------------------|------------------|------------------|------------------|-------------|-------------------------|----------------------------|
|                                                            | Polybutylene extrusion | Polypropylene    |                  |                  | Polyallomer | Injection molding       | 40% glass-fiber-reinforced |
|                                                            |                        | Homopolymer      | Copolymer        | Impact copolymer |             |                         |                            |
| <u>Physical</u>                                            |                        |                  |                  |                  |             |                         |                            |
| Melting temperature, °C                                    | 126                    | 168              | 160–168          |                  | 120–135     | 290                     | 290                        |
| Crystalline                                                |                        |                  |                  |                  |             |                         |                            |
| Amorphous                                                  |                        |                  |                  |                  |             |                         |                            |
| Specific gravity                                           | 0.91–0.925             | 0.90–0.91        | 0.89–0.905       | 0.90             | 0.90        | 1.3                     | 1.6                        |
| Water absorption (24 h),%                                  | 0.01–0.02              | 0.01–0.03        | 0.03             | <0.03            | <0.01       | <0.02                   | 0.05                       |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 18                     | 24               | 24               | 24               | 31          | 15                      | 18                         |
| <u>Electrical</u>                                          |                        |                  |                  |                  |             |                         |                            |
| Volume (dc) resistivity, ohm-cm                            |                        | 10 <sup>17</sup> | 10 <sup>17</sup> | 10 <sup>17</sup> |             |                         |                            |
| Dielectric constant (60 Hz)                                |                        | 2.2–2.6          | 2.3              |                  |             |                         |                            |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                        | 2.2–2.6          | 2.3              | 2.3              |             |                         |                            |
| Dissipation (power) factor (60 Hz)                         |                        | <0.0005          | 0.0001–0.0005    |                  |             |                         |                            |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                        | 0.0005–0.002     | 0.0001–0.0002    | 0.0003           |             |                         |                            |
| <u>Mechanical</u>                                          |                        |                  |                  |                  |             |                         |                            |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> | 31                     | 150–300          |                  |                  |             |                         |                            |



**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Polyolefin             |               |           |                                                    |             | Poly(phenylene sulfide) |                            |
|------------------------------------------------------------------------------------------|------------------------|---------------|-----------|----------------------------------------------------|-------------|-------------------------|----------------------------|
|                                                                                          | Polybutylene extrusion | Polypropylene |           |                                                    | Polyallomer | Injection molding       | 40% glass-fiber-reinforced |
|                                                                                          |                        | Homopolymer   | Copolymer | Impact copolymer                                   |             |                         |                            |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 300–380                | 5.5–8.0       | 3.5–8.0   | 8–20                                               | 400–500     | 16                      | 21                         |
| Elongation at break, %                                                                   |                        | 100–600       | 200–700   |                                                    |             | 1–2                     | 1                          |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 45–50                  | 170–250       | 130–200   | 130–190                                            | 70–110      | 550                     | 1700                       |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              | 2–2.3                  | 6–8           | 5–7       | R40–R90                                            | R50–R85     | 14                      | 29                         |
| Hardness, Rockwell (or Shore)                                                            |                        | R80–R102      | R50–R96   |                                                    |             | R123                    | R123                       |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | No break               | 21–53         | 53–1068   | 80–900                                             | 91–203      | <27                     | 75                         |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  | 30–40                  | 165–225       | 100–170   |                                                    |             | 480                     | 1100                       |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 3.8–4.4                | 4.5–6         | 4–5.5     |                                                    | 3–3.8       | 9.5                     | 19.5                       |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           | 1.7–2.5                | 4.5–5.4       | 3.5–4.3   | 2.5–3.1                                            | 3–3.4       |                         |                            |
| <u>Thermal</u>                                                                           |                        |               |           |                                                    |             |                         |                            |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          |                        |               |           |                                                    |             |                         |                            |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                        | 128–150                | 81–100        | 68–95     | 60–90                                              | 83–100      | 49                      | 22                         |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C | 54–60                  | 48–57         | 45–57     | 90–105<br>( $66 \text{ lb} \cdot \text{in}^{-2}$ ) | 51–56       | 135                     | 249                        |
| Maximum recommended service temperature, °C                                              |                        | 160           | 240       | 140–160                                            |             |                         |                            |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          |                        | 0.44–0.46     | 0.45–0.50 | 0.45–0.50                                          |             |                         |                            |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.22                   | 0.12          | 0.15–0.17 | 0.12–0.17                                          | 0.09–0.17   | 0.29                    | 0.29                       |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Polyurethane                       |             |                                    | Silicone                           |                             |                                          | Styrenic           |
|------------------------------------------------------------|------------------------------------|-------------|------------------------------------|------------------------------------|-----------------------------|------------------------------------------|--------------------|
|                                                            | Casting resin                      |             | Thermoplastic elastomer            | Cast resin, flexible               | Mineral-and/or glass-filled | Epoxy molding and encapsulating compound | Polystyrene        |
|                                                            | Liquid                             | Unsaturated |                                    |                                    |                             |                                          | Crystal            |
| <u>Physical</u>                                            |                                    |             |                                    |                                    |                             |                                          |                    |
| Melting temperature, °C                                    |                                    |             |                                    |                                    |                             |                                          |                    |
| Crystalline                                                | Thermoset                          | Thermoset   |                                    | Thermoset                          | Thermoset                   | Thermoset                                | 85–105             |
| Amorphous                                                  |                                    |             | 120–160                            |                                    |                             |                                          |                    |
| Specific gravity                                           | 1.1–1.5                            | 1.05        | 1.05–1.25                          | 0.99–1.5                           | 1.8–1.94                    | 1.84                                     | 1.04–1.05          |
| Water absorption (24 h), %                                 | 0.02–1.5                           | 0.1–0.2     | 0.7–0.9                            |                                    |                             |                                          | 0.03–0.10          |
| Dielectric strength, kV · mm <sup>-1</sup>                 | 12–20                              |             | 13–25                              | 22                                 | 8–15                        | 10                                       | 24                 |
| <u>Electrical</u>                                          |                                    |             |                                    |                                    |                             |                                          |                    |
| Volume (dc) resistivity, ohm-cm                            | 10 <sup>11</sup> –10 <sup>15</sup> |             | 10 <sup>11</sup> –10 <sup>13</sup> | 10 <sup>14</sup> –10 <sup>15</sup> |                             |                                          | > 10 <sup>16</sup> |
| Dielectric constant (60 Hz)                                | 4.0–7.5                            |             | 5.4–7.6                            | 2.7–4.2                            |                             |                                          |                    |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                                    |             |                                    |                                    |                             |                                          | 2.5                |
| Dissipation (power) factor (60 Hz)                         |                                    |             |                                    |                                    |                             |                                          |                    |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                                    |             |                                    |                                    |                             |                                          |                    |
| <u>Mechanical</u>                                          |                                    |             |                                    |                                    |                             |                                          |                    |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>-2</sup> | 10–100                             |             | 4–9                                |                                    |                             |                                          |                    |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Polyurethane           |             |                         | Silicone             |                             |                                          | Styrenic        |
|------------------------------------------------------------------------------------------|------------------------|-------------|-------------------------|----------------------|-----------------------------|------------------------------------------|-----------------|
|                                                                                          | Casting resin          |             | Thermoplastic elastomer | Cast resin, flexible | Mineral-and/or glass-filled | Epoxy molding and encapsulating compound | Polystyrene     |
|                                                                                          | Liquid                 | Unsaturated |                         |                      |                             |                                          | Crystal         |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 20                     |             | 20                      |                      | 10–16                       | 28                                       | 11.5–16         |
| Elongation at break, %                                                                   | 100–1000               | 3–6         | 100–1100                | 100–700              |                             |                                          | 1–2             |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 10–100                 | 610         | 10–350                  |                      | 1000–2500                   |                                          | 380–450         |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              | 0.7–4.5                | 19          | 0.7–9<br>(A65–D80)      | (A15–A65)            | 9–14<br>M80–M90             | 17                                       | 8–14<br>M60–M75 |
| Hardness, Rockwell (or Shore)                                                            |                        |             |                         |                      |                             |                                          |                 |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | 1334 to flexible       | 21          | No break                |                      | 13–427                      | 16                                       | 13–21           |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  | 10–100                 |             | 10–350                  |                      |                             |                                          | 350–485         |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 0.175–10               | 10–11       | 1.5–8.4                 | 0.35–1.0             | 4–6.5                       | 6–8                                      | 5.3–7.9         |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                        |             |                         |                      |                             |                                          |                 |
| <u>Thermal</u>                                                                           |                        |             |                         |                      |                             |                                          |                 |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          |                        |             |                         |                      | 0–78                        |                                          |                 |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                        | 100–200                |             | 100–200                 | 300–800              | 20–50                       | 30                                       | 70–80           |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C | Varies over wide range | 87–93       | Varies over wide range  |                      | 260                         | 74–100                                   |                 |
| Maximum recommended service temperature, °C                                              |                        |             |                         |                      | 371                         |                                          | 93              |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          | 0.43                   |             | 0.43                    |                      |                             |                                          | 0.3             |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.21                   |             | 0.07–0.31               | 0.15–0.31            | 0.30                        | 0.68                                     | 0.09–0.13       |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Styrenic       |                                           |                |             |                |           |                      |
|------------------------------------------------------------|----------------|-------------------------------------------|----------------|-------------|----------------|-----------|----------------------|
|                                                            | Polystyrene    | Acrylonitrile-butadiene-styrene copolymer |                |             |                |           |                      |
|                                                            | Heat-resistant | Extrusion                                 | Molding        |             |                |           |                      |
|                                                            |                |                                           | Heat-resistant | High-impact | Flame-retarded | Platable  | 20% glass-reinforced |
| <u>Physical</u>                                            |                |                                           |                |             |                |           |                      |
| Melting temperature, °C                                    |                |                                           |                |             |                |           |                      |
| Crystalline                                                |                |                                           |                |             |                |           |                      |
| Amorphous                                                  | 110–125        | 88–120                                    | 110–125        | 100–110     | 110–125        | 100–110   |                      |
| Specific gravity                                           | 1.05–1.09      | 1.02–1.06                                 | 1.05–1.08      | 1.01–1.04   | 1.16–1.21      | 1.06–1.07 | 1.22                 |
| Water absorption (24 h), %                                 | 0.03–0.12      | 0.20–0.45                                 | 0.20–0.45      | 0.20–0.45   | 0.2–0.6        |           |                      |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 20             | 14–20                                     | 14–20          | 14–20       | 14–20          | 16–22     | 18                   |
| <u>Electrical</u>                                          |                |                                           |                |             |                |           |                      |
| Volume (dc) resistivity, ohm-cm                            |                |                                           |                |             |                |           |                      |
| Dielectric constant (60 Hz)                                |                |                                           |                | 2.4–5.0     |                |           |                      |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                |                                           |                | 2.4–3.8     |                |           |                      |
| Dissipation (power) factor (60 Hz)                         |                |                                           |                | 0.003–0.008 |                |           |                      |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                |                                           |                | 0.007–0.015 |                |           |                      |
| <u>Mechanical</u>                                          |                |                                           |                |             |                |           |                      |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> |                | 150–390                                   | 190–440        | 140–300     | 130–310        |           |                      |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                             | Styrenic       |                 |                                           |                 |                 |                 |                      |
|----------------------------------------------------------------------------------------|----------------|-----------------|-------------------------------------------|-----------------|-----------------|-----------------|----------------------|
|                                                                                        | Heat-resistant | Extrusion       | Acrylonitrile-butadiene-styrene copolymer |                 |                 |                 |                      |
|                                                                                        |                |                 | Molding                                   |                 |                 |                 |                      |
|                                                                                        |                |                 | Heat-resistant                            | High-impact     | Flame-retarded  | Platable        | 20% glass-reinforced |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$      | 11.5–16        | 5.2–10          | 7.2–10                                    | 4.5–8           | 6.5–7.5         |                 | 14                   |
| Elongation at break, %                                                                 | 2–60           | 20–100          | 3–20                                      | 5–70            | 5–25            |                 |                      |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                       | 340–470        | 130–420         | 300–400                                   | 250–350         | 300–400         | 340–390         | 710                  |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$            | 8.9–14         | 4–14            | 10–13                                     | 8–11            | 9–14            | 10.5–11.5       | 15.5                 |
| Hardness, Rockwell (or Shore)                                                          | L80–L108       | R75–R115        | R100–R115                                 | R85–R105        | R100–R120       | R103–R109       | M85                  |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                         | 21–181         | 133–640         | 107–347                                   | 347–400         | 160–640         | 267–283         | 64                   |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                | 320–460        | 130–380         | 300–350                                   | 230–330         | 320–400         | 330–380         | 740                  |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                      | 5–7.8          | 2.5–8.0         | 6–7.5                                     | 4.8–6.3         | 5–8             | 6–6.4           | 11                   |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         |                |                 | 5.5–7                                     | 4–5.5           | 4–6             |                 |                      |
| Thermal                                                                                |                |                 |                                           |                 |                 |                 |                      |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                        |                | 1.3             |                                           | 1.3             |                 |                 |                      |
| Coefficient of linear thermal expansion, $10^{-6}^\circ\text{C}$                       | 60–70          | 60–130          | 60–93                                     | 95–110          | 65–95           | 47–53           | 21                   |
| Deflection temperature under flexural load (264 $\text{lb} \cdot \text{in}^{-2}$ ), °C | 93–120         | 77–104 annealed | 104–116 annealed                          | 96–102 annealed | 90–107 annealed | 96–102 annealed | 99                   |
| Maximum recommended service temperature, °C                                            |                |                 |                                           | 110             |                 |                 |                      |
| Specific heat, $\text{cal g}^{-1}$                                                     |                |                 |                                           | 0.3–0.4         |                 |                 |                      |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$               |                |                 | 0.19–0.34                                 |                 |                 |                 |                      |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Styrenic                        |                            |                                          | Sulfone          |                            |                     | Poly(phenyl sulfone) |
|------------------------------------------------------------|---------------------------------|----------------------------|------------------------------------------|------------------|----------------------------|---------------------|----------------------|
|                                                            | Styrene-acrylonitrile copolymer |                            | Styrene-butadiene copolymer, high-impact | Polysulfone      |                            | Poly(ether sulfone) |                      |
|                                                            | Unfilled                        | 20% glass-fiber-reinforced |                                          | Unfilled         | 20% glass-fiber-reinforced |                     |                      |
| <u>Physical</u>                                            |                                 |                            |                                          |                  |                            |                     |                      |
| Melting temperature, °C                                    |                                 |                            |                                          |                  |                            |                     |                      |
| Crystalline                                                |                                 |                            |                                          |                  |                            |                     |                      |
| Amorphous                                                  | 115–125                         | 115–125                    | 90–110                                   | 200              | 200                        | 230                 | 220                  |
| Specific gravity                                           | 1.07–1.08                       | 1.22                       | 1.03–1.06                                | 1.24             | 1.46                       | 1.37                | 1.29                 |
| Water absorption (24 h), %                                 | 0.2–0.3                         | 0.15–0.20                  | 0.05–0.10                                | 0.22             | 0.23                       | 0.43                | 1.1–1.3 (saturated)  |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 16–20                           | 20                         | 18                                       | 17               | 17                         | 17                  | 16                   |
| <u>Electrical</u>                                          |                                 |                            |                                          |                  |                            |                     |                      |
| Volume (dc) resistivity, ohm-cm                            |                                 |                            |                                          | 10 <sup>15</sup> |                            |                     |                      |
| Dielectric constant (60 Hz)                                |                                 |                            |                                          | 3.14             | 3.7                        |                     |                      |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                                 |                            |                                          | 3.26             | 3.7                        |                     |                      |
| Dissipation (power) factor (60 Hz)                         |                                 |                            |                                          | 0.004            | 0.002                      |                     |                      |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                                 |                            |                                          | 0.008            | 0.009                      |                     |                      |
| <u>Mechanical</u>                                          |                                 |                            |                                          |                  |                            |                     |                      |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> | 530                             |                            |                                          | 370              |                            |                     |                      |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Styrenic                        |                            |                                          | Sulfone     |                            |                     | Poly(phenyl sulfone) |
|------------------------------------------------------------------------------------------|---------------------------------|----------------------------|------------------------------------------|-------------|----------------------------|---------------------|----------------------|
|                                                                                          | Styrene-acrylonitrile copolymer |                            | Styrene-butadiene copolymer, high-impact | Polysulfone |                            | Poly(ether sulfone) |                      |
|                                                                                          | Unfilled                        | 20% glass-fiber-reinforced |                                          | Unfilled    | 20% glass-fiber-reinforced |                     |                      |
| Compressive strength, rupture of 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 14–17                           | 19                         | 4–9                                      | 13.9        | 22                         |                     |                      |
| Elongation at break, %                                                                   | 1–4                             | 1–2                        | 13–50                                    | 50–100      | 2                          | 30–80               | 60                   |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 550                             | 100–1100                   | 280–450                                  | 390         | 1000                       | 375                 | 330                  |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              | 14–17                           | 20                         | 5.3–9.4                                  | 15.4        | 23                         | 18.7                | 12.4                 |
| Hardness, Rockwell (or Shore)                                                            | M80–M90                         | R122                       | M10–M68                                  | M69, R120   | M123                       | M88                 |                      |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | 19–27                           | 53                         | 32–192                                   | 64          | 59                         | 85                  | 640                  |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  | 400–560                         | 1150–1200                  | 280–465                                  | 360         | 1200                       | 350                 | 310                  |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 9–12                            | 15.8–18                    | 3.2–4.9                                  |             | 17                         |                     |                      |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                                 |                            | 2.9–4.9                                  | 10.2        |                            | 12.2                | 10.4                 |
| Thermal                                                                                  |                                 |                            |                                          |             |                            |                     |                      |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          |                                 |                            |                                          |             |                            |                     |                      |
| Coefficient of linear thermal expansion, $10^{-6}^\circ\text{C}$                         | 36–38                           | 38–40                      | 70–101                                   | 52–56       | 25                         | 55                  | 31                   |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C | 88–104                          | 99                         | 74–93                                    | 174         | 182                        | 203                 | 204                  |
| Maximum recommended service temperature, °C                                              |                                 |                            |                                          | 149         |                            |                     |                      |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          |                                 |                            |                                          |             |                            |                     |                      |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.12                            | 0.26–0.28                  | 0.12–0.21                                | 0.12        | 0.38                       | 0.14–0.19           |                      |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Thermoplastic elastomers |           |                                                                   |                                                                  | Urea formaldehyde, alpha-cellulose filled | Vinyl                                        |                                    |
|------------------------------------------------------------|--------------------------|-----------|-------------------------------------------------------------------|------------------------------------------------------------------|-------------------------------------------|----------------------------------------------|------------------------------------|
|                                                            | Polyolefin               | Polyester | Block copolymers of styrene and butadiene or styrene and isoprene | Block copolymers of styrene and ethylene or styrene and butylene |                                           | Poly(vinyl chloride) and poly(vinyl acetate) |                                    |
|                                                            |                          |           |                                                                   |                                                                  |                                           | Rigid                                        | Flexible and unfilled              |
| <u>Physical</u>                                            |                          |           |                                                                   |                                                                  |                                           |                                              |                                    |
| Melting temperature, °C                                    |                          |           |                                                                   |                                                                  | Thermoset                                 |                                              |                                    |
| Crystalline                                                |                          | 168–206   |                                                                   |                                                                  |                                           |                                              |                                    |
| Amorphous                                                  |                          |           |                                                                   |                                                                  |                                           | 75–105                                       | 75–105                             |
| Specific gravity                                           | 0.88–0.90                | 1.17–1.25 | 0.9–1.2                                                           | 0.9–1.2                                                          | 1.47–1.52                                 | 1.30–1.58                                    | 1.16–1.35                          |
| Water absorption (24 h), %                                 | 0.01                     |           | 0.19–0.39                                                         |                                                                  | 0.4–0.8                                   | 0.04–0.4                                     | 0.15–0.75                          |
| Dielectric strength, kV · mm <sup>−1</sup>                 | 24–26                    |           | 16–21                                                             |                                                                  | 12–16                                     | 14–20                                        | 12–16                              |
| <u>Electrical</u>                                          |                          |           |                                                                   |                                                                  |                                           |                                              |                                    |
| Volume (dc) resistivity, ohm-cm                            |                          |           |                                                                   |                                                                  | 0.5–5.0                                   | 10 <sup>12</sup> –10 <sup>15</sup>           | 10 <sup>11</sup> –10 <sup>14</sup> |
| Dielectric constant (60 Hz)                                |                          |           |                                                                   |                                                                  | 7.7–9.5                                   | 3.2–4.0                                      | 5.0–9.0                            |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                          |           |                                                                   |                                                                  | 6.7–8.0                                   | 3.0–4.0                                      | 3.0–4.0                            |
| Dissipation (power) factor (60 Hz)                         |                          |           |                                                                   |                                                                  | 0.036–0.043                               | 0.01–0.02                                    | 0.03–0.05                          |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                          |           |                                                                   |                                                                  | 0.025–0.035                               | 0.006–0.02                                   | 0.06–0.1                           |
| <u>Mechanical</u>                                          |                          |           |                                                                   |                                                                  |                                           |                                              |                                    |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>−2</sup> |                          |           | 3.6–120                                                           |                                                                  |                                           |                                              |                                    |



**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                                               | Thermoplastic elastomers |                 |                                                                   |                                                                  | Urea formaldehyde, alpha-cellulose filled | Vinyl                                        |                            |
|------------------------------------------------------------------------------------------|--------------------------|-----------------|-------------------------------------------------------------------|------------------------------------------------------------------|-------------------------------------------|----------------------------------------------|----------------------------|
|                                                                                          | Polyolefin               | Polyester       | Block copolymers of styrene and butadiene or styrene and isoprene | Block copolymers of styrene and ethylene or styrene and butylene |                                           | Poly(vinyl chloride) and poly(vinyl acetate) |                            |
|                                                                                          |                          |                 |                                                                   |                                                                  |                                           | Rigid                                        | Flexible and unfilled      |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 150–300                  | 350–450         | 500–1350                                                          | 600–800                                                          | 25–45                                     | 8–13                                         | 0.9–1.7                    |
| Elongation at break, %                                                                   |                          |                 |                                                                   |                                                                  | <1                                        | 40–80                                        | 200–450                    |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         | 1.5–2.0                  | 7–75            | 4–150                                                             | 4–100                                                            | 1300–1600                                 | 300–500                                      |                            |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              |                          |                 |                                                                   |                                                                  | 10–18                                     | 10–16                                        |                            |
| Hardness, Rockwell (or Shore)                                                            | (A65–A92)                | (D40–D72)       | (A40–A90)                                                         | (A50–A90)                                                        | M110–M120                                 | (D65–D95)                                    | (A50–A100)                 |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | No break                 | 208 to no break | No break                                                          | No break                                                         | 13–21                                     | 21–1068                                      | Varies over wide range     |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  |                          | 1.1–2.5         | 0.8–50                                                            |                                                                  | 1000–1500                                 | 350–600                                      |                            |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 0.65–2.0                 | 3.7–5.7         | 0.6–3.0                                                           | 1–3                                                              | 5.5–13                                    | 6–75                                         | 1.5–3.5                    |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                          |                 |                                                                   |                                                                  |                                           |                                              |                            |
| <u>Thermal</u>                                                                           |                          |                 |                                                                   |                                                                  |                                           |                                              |                            |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          |                          |                 |                                                                   |                                                                  | Self-extinguishing                        | Self-extinguishing                           | Slow to self-extinguishing |
| Coefficient of linear thermal expansion, $10^{-6}\text{°C}$                              | 130–170                  |                 | 130–137                                                           |                                                                  | 22–36                                     | 50–100                                       | 70–250                     |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C |                          |                 | <0–49                                                             |                                                                  | 127–143                                   | 60–77                                        |                            |
| Maximum recommended service temperature, °C                                              |                          |                 |                                                                   |                                                                  | 77                                        | 70–74                                        | 80–105                     |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          |                          |                 |                                                                   |                                                                  | 0.6                                       | 0.2–0.28                                     | 0.36–0.5                   |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.19–0.21                |                 | 0.15                                                              |                                                                  | 0.30–0.42                                 | 0.15–0.21                                    | 0.13–0.17                  |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

| Properties                                                 | Vinyl                                        |                                                  |                                    |                    |                                  |                               |  |
|------------------------------------------------------------|----------------------------------------------|--------------------------------------------------|------------------------------------|--------------------|----------------------------------|-------------------------------|--|
|                                                            | Poly(vinyl chloride) and poly(vinyl acetate) | Poly(vinyl chloride), 15% glass-fiber-reinforced | Poly(vinylidene chloride)          | Poly(vinyl formal) | Chlorinated poly(vinyl chloride) | Poly(vinyl butyral), flexible |  |
|                                                            | Flexible and filled                          |                                                  |                                    |                    |                                  |                               |  |
| <u>Physical</u>                                            |                                              |                                                  |                                    |                    |                                  |                               |  |
| Melting temperature, °C                                    |                                              |                                                  |                                    |                    |                                  |                               |  |
| Crystalline                                                |                                              |                                                  | 210                                |                    |                                  |                               |  |
| Amorphous                                                  | 75–105                                       | 75–105                                           |                                    | 105                | 110                              | 49                            |  |
| Specific gravity                                           | 1.3–1.7                                      | 1.54                                             | 1.65–1.72                          | 1.2–1.4            | 1.49–1.56                        | 1.05                          |  |
| Water absorption (24 h),%                                  | 0.5–1.0                                      | 0.01                                             | 0.1                                | 0.5–3.0            | 0.02–0.15                        | 1.0–2.0                       |  |
| Dielectric strength, kV · mm <sup>-1</sup>                 | 9.8–12                                       | 24–31                                            | 16–24                              | 19                 |                                  | 14                            |  |
| <u>Electrical</u>                                          |                                              |                                                  |                                    |                    |                                  |                               |  |
| Volume (dc) resistivity, ohm-cm                            |                                              |                                                  | 10 <sup>14</sup> –10 <sup>16</sup> |                    |                                  |                               |  |
| Dielectric constant (60 Hz)                                |                                              |                                                  | 4.5–6.0                            |                    |                                  |                               |  |
| Dielectric constant (10 <sup>6</sup> Hz)                   |                                              |                                                  |                                    |                    |                                  |                               |  |
| Dissipation (power) factor (60 Hz)                         |                                              |                                                  |                                    |                    |                                  |                               |  |
| Dissipation factor (10 <sup>6</sup> Hz)                    |                                              |                                                  |                                    |                    |                                  |                               |  |
| <u>Mechanical</u>                                          |                                              |                                                  |                                    |                    |                                  |                               |  |
| Compressive modulus, 10 <sup>3</sup> lb · in <sup>-2</sup> |                                              |                                                  |                                    |                    | 335–600                          |                               |  |

**TABLE 10.2** Properties of Commercial Plastics (*Continued*)

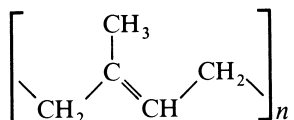
| Properties                                                                               | Vinyl                                        |                                                  |                           |                    |                                  |                               |  |
|------------------------------------------------------------------------------------------|----------------------------------------------|--------------------------------------------------|---------------------------|--------------------|----------------------------------|-------------------------------|--|
|                                                                                          | Poly(vinyl chloride) and poly(vinyl acetate) | Poly(vinyl chloride), 15% glass-fiber-reinforced | Poly(vinylidene chloride) | Poly(vinyl formal) | Chlorinated poly(vinyl chloride) | Poly(vinyl butyral), flexible |  |
|                                                                                          | Flexible and filled                          |                                                  |                           |                    |                                  |                               |  |
| Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$        | 1.0–1.8                                      | 9                                                | 2–2.7                     |                    | 9–22                             |                               |  |
| Elongation at break, %                                                                   | 200–400                                      | 2–3                                              | 50–250                    | 5–20               | 4–65                             | 150–450                       |  |
| Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$                         |                                              | 750                                              |                           |                    | 380–450                          |                               |  |
| Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$              |                                              | 13.5                                             | 4.2–6.2                   | 17–18              | 14.5–17                          |                               |  |
| Hardness, Rockwell (or Shore)                                                            | (A50–A100)                                   | R118                                             | M50–M65                   | M85                | R117–R122                        | A10–A100                      |  |
| Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$                           | Varies over wide range                       | 53                                               | 16–53                     | 43–75              | 53–299                           | Varies over wide range        |  |
| Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$                                  |                                              | 870                                              | 50–80                     | 350–600            | 360–475                          |                               |  |
| Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$                        | 1–3.5                                        | 9.5                                              | 3–5                       | 10–12              | 7.5–9                            | 0.5–3.0                       |  |
| Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$                           |                                              |                                                  |                           |                    |                                  |                               |  |
| Thermal                                                                                  |                                              |                                                  |                           |                    |                                  |                               |  |
| Burning rate, $\text{mm} \cdot \text{min}^{-1}$                                          |                                              |                                                  | Self-extinguishing        |                    |                                  | Slow                          |  |
| Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$                        |                                              |                                                  | 190                       | 64                 | 68–78                            |                               |  |
| Deflection temperature under flexural load ( $264 \text{ lb} \cdot \text{in}^{-2}$ ), °C |                                              | 68                                               | 54–71                     | 71–77              | 94–112                           |                               |  |
| Maximum recommended service temperature, °C                                              |                                              |                                                  | 100                       |                    |                                  |                               |  |
| Specific heat, $\text{cal} \cdot \text{g}^{-1}$                                          |                                              |                                                  | 0.32                      |                    |                                  |                               |  |
| Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$                 | 0.13–0.17                                    |                                                  | 0.13                      | 0.16               | 0.14                             |                               |  |

## 10.4 FORMULAS AND ADVANTAGES OF RUBBERS

---

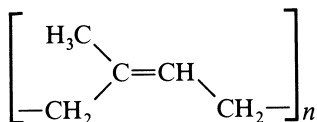
### 10.4.1 Gutta Percha

Gutta percha is a natural polymer of isoprene (3-methyl-1,3-butadiene) in which the configuration around each double bond is *trans*. It is hard and horny and has the following formula:



### 10.4.2 Natural Rubber

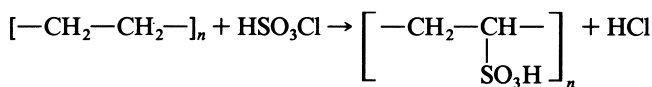
Natural rubber is a polymer of isoprene in which the configuration around each double bond is *cis* (or *Z*):



Its principal advantages are high resilience and good abrasion resistance.

### 10.4.3 Chlorosulfonated Polyethylene

Chlorosulfonated polyethylene is prepared as follows:



Cross-linking, which can occur as a result of side reactions, causes an appreciable gel content in the final product.

The polymer can be vulcanized to give a rubber with very good chemical (solvent) resistance, excellent resistance to aging and weathering, and good color retention in sunlight.

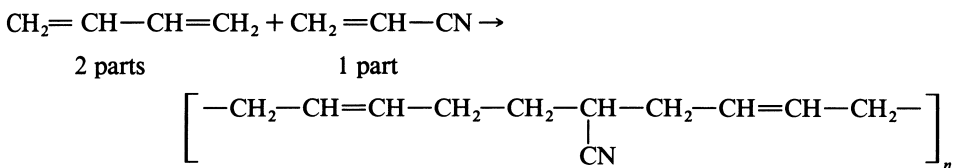
#### 10.4.4 Epichlorohydrin

Epichlorohydrin is a product of covulcanization of epichlorohydrin (epoxy) polymers with rubbers, especially *cis*-polybutadiene.

Its advantages include impermeability to air, excellent adhesion to metal, and good resistance to oils, weathering, and low temperature.

#### 10.4.5 Nitrile Rubber (NBR, GRN, Buna N)

Nitrile rubber can be prepared as follows:

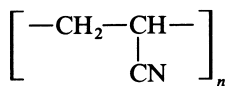


Nitrile rubber is also known as nitrile-butadiene rubber (NBR), government rubber nitrile (GRN), and Buna N.

It possesses resistance to oils up to 120°C and excellent abrasion resistance and adhesion to metal.

#### 10.4.6 Polyacrylate

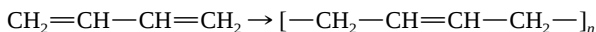
Polyacrylate has the following formula:



It possesses oil and heat resistance to 175°C and excellent resistance to ozone.

#### 10.4.7 *cis*-Polybutadiene Rubber (BR)

*cis*-Polybutadiene is prepared by polymerization of butadiene by mostly 1,4-addition.

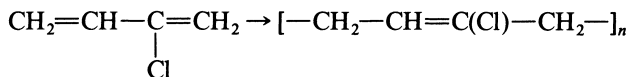


The polybutadiene produced is in the *Z* (or *cis*) configuration.

*cis*-Polybutadiene has good abrasion resistance, is useful at low temperature, and has excellent adhesion to metal.

### 10.4.8 Polychloroprene (Neoprene)

Polychloroprene is prepared as follows:



It has very good weathering characteristics, is resistant to ozone and to oil, and is heat-resistant to 100°C.

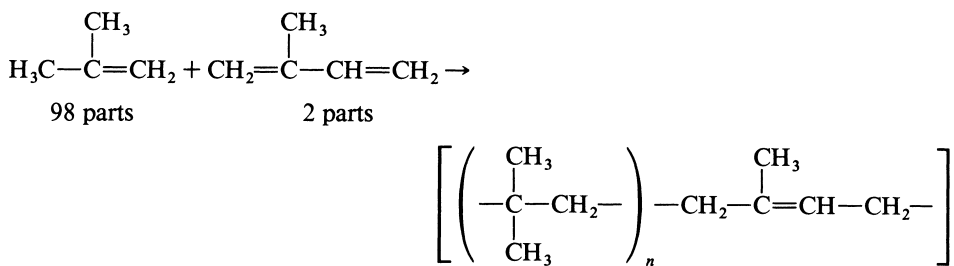
### 10.4.9 Ethylene-Propylene-Diene Rubber (EPDM)

Ethylene-propylene-diene rubber is polymerized from 60 parts ethylene, 40 parts propylene, and a small amount of nonconjugated diene. The nonconjugated diene permits sulfur vulcanization of the polymer instead of using peroxide.

It is a very lightweight rubber and has very good weathering and electrical properties, excellent adhesion, and excellent ozone resistance.

### 10.4.10 Polyisobutylene (Butyl Rubber)

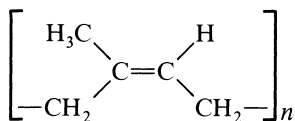
Polyisobutylene is prepared as follows:



It possesses excellent ozone resistance, very good weathering and electrical properties, and good heat resistance.

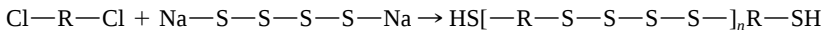
### 10.4.11 (Z)-Polyisoprene (Synthetic Natural Rubber)

Polymerization of isoprene by 1,4-addition produces polyisoprene that has a *cis* (or *Z*) configuration.



### 10.4.12 Polysulfide Rubbers

Polysulfide rubbers are prepared as follows:



where R can be



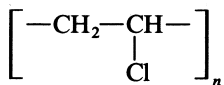
or



Polysulfide rubbers possess excellent resistance to weathering and oils and have very good electrical properties.

### 10.4.13 Poly(vinyl Chloride) (PVC)

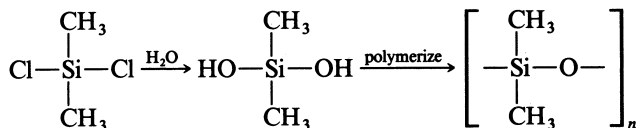
Poly(vinyl chloride) as previously discussed in Sec. 10.3, Formulas and Key Properties of Plastic Materials, has the following structures:



PVC polymer plus special plasticizers are used to produce flexible tubing which has good chemical resistance.

### 10.4.14 Silicone Rubbers

Silicone rubbers are prepared as follows:

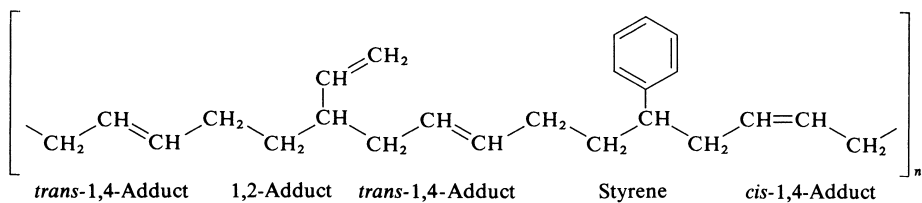


Other groups may replace the methyl groups.

Silicone rubbers have excellent ozone and weathering resistance, good electrical properties, and good adhesion to metal.

### 10.4.15 Styrene-Butadiene Rubber (GRS, SBR, Buna S)

Styrene-butadiene rubber is prepared from the free-radical copolymerization of one part by weight of styrene and three parts by weight of 1,3-butadiene. The butadiene is incorporated by both 1,4-addition (80%) and 1,2-addition (20%). The configuration around the double bond of the 1,4-adduct is about 80% *trans*. The product is a random copolymer with these general features:



Styrene-butadiene rubber (SBR) is also known as government rubber styrene (GRS) and Buna S.

#### 10.4.16 Urethane

See Table 10.3.



**TABLE 10.3** Properties of Natural and Synthetic Rubbers

| Rubber                                                                         | Specific gravity | Durometer hardness (or Shore) | Ultimate elongation % (23°C) | Tensile strength, lb · in <sup>-2</sup> (23°C) | Service temperature, °C |         |
|--------------------------------------------------------------------------------|------------------|-------------------------------|------------------------------|------------------------------------------------|-------------------------|---------|
|                                                                                |                  |                               |                              |                                                | Minimum                 | Maximum |
| Gutta percha (hard rubber)                                                     | 1.2–1.95         | (65–95)                       | 3–8                          | 4000–10,000                                    |                         | 104     |
| Natural rubber (NR)                                                            | 0.93             | 20–100                        | 750–850                      | 3000–4500                                      | –56                     | 82      |
| Chlorosulfonated polyethylene                                                  | 1.10             | 50–95                         | 100–500                      | 500–3000                                       | –54                     | 121     |
| Epichlorohydrin                                                                | 1.27             | 60–90                         | 100–400                      | 1000–2500                                      | –46                     | 121     |
| Fluoroelastomers                                                               | 1.4–1.95         | 60–90                         | 100–350                      | 2000–3000                                      | –40                     | 232     |
| Isobutene-isoprene rubber (IIR) [also known as government rubber I (GR-I)]     | 0.91             | (40–70)                       | 750–950                      | 2300–3000                                      |                         | 121     |
| Nitrile rubber (butadiene-acrylonitrile rubber) (also known as Buna N and NBR) | 1.00             | 30–100                        | 100–600                      | 500–4000                                       | –54                     | 121     |
| Polyacrylate                                                                   | 1.10             | 40–100                        | 100–400                      | 1000–2200                                      | –18                     | 149     |
| Polybutadiene rubber (BR)                                                      | 0.93             | 30–100                        | 100–700                      | 2500–3000                                      | –62                     | 79–100  |
| Polychloroprene (neoprene)                                                     | 1.23             | 20–90                         | 800–1000                     | 2000–3500                                      | –54                     | 121     |
| Poly(ethylene-propylene-diene) (EPDM)                                          | 0.85             | 30–100                        | 100–300                      | 1000–3000                                      | –40                     | 149     |
| Polyisobutylene (butyl rubber)                                                 | 0.92             | 30–100                        | 100–700                      | 1000–3000                                      | –54                     | 100     |
| Polyisoprene                                                                   | 0.94             | 20–100                        | 100–750                      | 2000–3000                                      | –54                     | 79–82   |
| Polysulfide (Thiokol ST)                                                       | 1.34             | 20–80                         | 100–400                      | 700–1250                                       | –54                     | 82–100  |
| Poly(vinyl chloride) (Koroseal)                                                | 1.32             | (80–90)                       |                              | 2400–3000                                      |                         | 71      |
| Silicone, high-temperature                                                     |                  |                               |                              | 700–800                                        |                         | 316     |
| Silicone                                                                       | 0.98             | 20–95                         | 50–800                       | 500–1500                                       | –84                     | 232     |
| Styrene-butadiene rubber (SBR) (also known as Buna S)                          | 0.94             | 40–100                        | 400–600                      | 1600–3700                                      | –60                     | 107     |
| Urethane                                                                       | 0.85             | 62–95                         | 100–700                      | 1000–8000                                      | –54                     | 100     |

10.5 CHEMICAL RESISTANCE

TABLE 10.4 Resistance of Selected Polymers and Rubbers to Various Chemicals at 20°C

The information in this table is intended to be used only as a general guide. The chemical resistance classifications are E = excellent (30 days of exposure causes no damage), G = good (some damage after 30 days), F = fair (exposure may cause crazing, softening, swelling, or loss of strength), N = not recommended (immediate damage may occur).

|                                                                                   | Chemical              |                                |                     |           |                        |        |        |         |                         |                        |                           |         |                          |
|-----------------------------------------------------------------------------------|-----------------------|--------------------------------|---------------------|-----------|------------------------|--------|--------|---------|-------------------------|------------------------|---------------------------|---------|--------------------------|
|                                                                                   | Acids, dilute or weak | Acids, strong and concentrated | Alcohols, aliphatic | Aldehydes | Alkalies, concentrated | Esters | Ethers | Glycols | Hydrocarbons, aliphatic | Hydrocarbons, aromatic | Hydrocarbons, halogenated | Ketones | Oxidizing agents, strong |
| Polymers                                                                          |                       |                                |                     |           |                        |        |        |         |                         |                        |                           |         |                          |
| Acetals                                                                           | F                     | N                              | F                   | N         | N                      | N      | N      | G       | N                       | N                      | N                         | N       | N                        |
| Acrylics: poly(methyl methacrylate)                                               | G                     | N                              | E                   | —         | N                      | N      | E      | E       | G                       | N                      | N                         | N       | N                        |
| Allyls: diallyl phthalate                                                         | G                     | —                              | —                   | —         | N                      | —      | —      | —       | E                       | G                      | G                         | N       | —                        |
| Cellulosics: cellulose-acetate-butyrate and cellulose-acetate-propionate polymers | F                     | N                              | N                   | N         | N                      | N      | N      | G       | F                       | N                      | N                         | N       | —                        |
| Fluorocarbons                                                                     | E                     | E                              | E                   | E         | E                      | E      | E      | E       | E                       | E                      | E                         | E       | E                        |
| Polyamides                                                                        | N                     | N                              | G                   | E         | E                      | G      | —      | G       | G                       | F                      | F                         | G       | N                        |
| Polycarbonates                                                                    | G                     | N                              | G                   | F         | N                      | N      | N      | G       | N                       | N                      | N                         | N       | N                        |
| Polyesters                                                                        | G                     | G                              | N                   | —         | N                      | N      | F      | G       | G                       | F                      | F                         | N       | F                        |
| Poly(methyl pentene)                                                              | E                     | E                              | G                   | G         | E                      | G      | N      | E       | F                       | G                      | N                         | F       | F                        |
| Low-density polyethylene                                                          | E                     | E                              | E                   | G         | E                      | G      | N      | E       | F                       | F                      | N                         | G       | F                        |
| High-density polyethylene                                                         | E                     | E                              | E                   | E         | E                      | G      | N      | E       | G                       | G                      | N                         | G       | F                        |
| Polybutadiene                                                                     | G                     | F                              | E                   | —         | —                      | —      | —      | —       | —                       | E                      | E                         | E       | —                        |

|  | Chemical              |                                |                     |           |                        |        |        |         |                         |                        |                           |         |                          |
|--|-----------------------|--------------------------------|---------------------|-----------|------------------------|--------|--------|---------|-------------------------|------------------------|---------------------------|---------|--------------------------|
|  | Acids, dilute or weak | Acids, strong and concentrated | Alcohols, aliphatic | Aldehydes | Alkalies, concentrated | Esters | Ethers | Glycols | Hydrocarbons, aliphatic | Hydrocarbons, aromatic | Hydrocarbons, halogenated | Ketones | Oxidizing agents, strong |

### Polymers

|                                            |   |   |   |   |   |   |   |   |   |   |   |   |   |
|--------------------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Polypropylene and polyallomer              | E | E | E | E | E | G | N | E | G | F | N | G | F |
| Polystyrene                                | N | N | E | — | N | N | — | E | N | N | N | N | N |
| Styrene-acrylonitrile copolymers           | — | — | N | — | N | — | — | F | N | — | — | — | — |
| Styrene-acrylonitrile-butadiene copolymers | — | N | G | — | G | N | — | — | F | N | N | N | — |
| Sulfones: polysulfone                      | G | N | F | F | E | N | F | G | F | N | N | N | G |
| Vinyls: poly(vinyl chloride)               | E | G | E | G | G | N | F | F | G | N | N | N | G |

### Rubbers

|                              |   |   |   |   |   |   |   |   |   |   |   |   |   |
|------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Natural rubber               | — | — | E | — | — | N | N | E | N | N | N | N | — |
| Nitrile rubber               | — | — | E | — | — | N | G | E | E | N | N | N | — |
| Polychloroprene              | — | — | E | — | — | N | F | E | F | N | N | N | — |
| Polyisobutylene              | — | — | E | — | — | F | F | E | N | N | N | N | — |
| Polysulfide rubbers: Thiokol | — | — | E | — | — | E | E | E | E | F | N | N | — |
| Styrene-butadiene rubber     | — | — | E | — | — | N | N | E | N | N | N | N | — |

TABLE 10.5 Gas Permeability Constants (10<sup>10</sup> P) at 25°C for Polymers and Rubbers

The gas permeability constant *P* is defined as

$$P = \frac{\text{amount of permeant}}{(\text{area}) \times (\text{time}) \times (\text{driving forced across the film})}$$

The gas permeability constant is the amount of gas expressed in cubic centimeters passed in 1 s through a 1-cm<sup>2</sup> area of film when the pressure across a film thickness of 1 cm is 1 cmHg and the temperature is 25°C. All tabulated values are multiplied by 10<sup>10</sup> and are in units of seconds<sup>-1</sup> (centimeters of Hg)<sup>-1</sup>. Other temperatures are indicated by exponents and are expressed in degrees Celsius.

| Polymer or rubber      | Gas                 |                       |                    |                     |                    |                      |                                                                                                                                                                             |
|------------------------|---------------------|-----------------------|--------------------|---------------------|--------------------|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                        | He                  | N <sub>2</sub>        | H <sub>2</sub>     | O <sub>2</sub>      | CO <sub>2</sub>    | H <sub>2</sub> O     | Other                                                                                                                                                                       |
| Cellulose (cellophane) | 0.005 <sup>20</sup> | 0.003 2               | 0.006 5            | 0.002 1             | 0.004 7            | 1 900                | 0.006 <sup>45</sup> (H <sub>2</sub> S); 0.001 7 (SO <sub>2</sub> )                                                                                                          |
| Cellulose acetate      | 13.6 <sup>20</sup>  | 0.28 <sup>30</sup>    | 3.5 <sup>20</sup>  | 0.78 <sup>30</sup>  | 22.7 <sup>30</sup> | 5 500                | 3.5 <sup>30</sup> (H <sub>2</sub> S); 17 <sup>0</sup> (ethylene oxide);<br>6.8 <sup>60</sup> (bromomethane)                                                                 |
| Cellulose nitrate      | 6.9                 | 0.12                  | 2.0 <sup>20</sup>  | 1.95                | 2.12               | 6 290                | 57.1 (NH <sub>3</sub> ); 1.76 (SO <sub>2</sub> )                                                                                                                            |
| Ethyl cellulose        | 400 <sup>30</sup>   | 8.4 <sup>30</sup>     | 87 <sup>20</sup>   | 26.5 <sup>30</sup>  | 41.0 <sup>30</sup> | 12 000 <sup>20</sup> | 705 (NH <sub>3</sub> ); 204 (SO <sub>2</sub> );<br>420 <sup>0</sup> (ethylene oxide)                                                                                        |
| Gutta percha           |                     | 2.17                  | 14.4               | 6.16                | 35.4               | 510                  |                                                                                                                                                                             |
| Natural rubber         |                     | 9.43                  | 52.0               | 23.3                | 15.3               | 2 290                | 15.7 (CO); 30.1 (CH <sub>4</sub> );<br>1.68 (C <sub>3</sub> H <sub>8</sub> ); 98.9 (C <sub>2</sub> H <sub>2</sub> );<br>550 (CH <sub>3</sub> C≡CH); 3.59 (SF <sub>6</sub> ) |
| Nylon 6                | 0.53 <sup>20</sup>  | 0.009 5 <sup>30</sup> |                    | 0.038 <sup>30</sup> | 0.10 <sup>30</sup> | 177                  | 0.33 <sup>30</sup> (H <sub>2</sub> S); 1.2 <sup>20</sup> (NH <sub>3</sub> );<br>0.84 <sup>60</sup> (CH <sub>3</sub> Br)                                                     |
| Nylon 11               | 1.95 <sup>30</sup>  |                       | 1.78 <sup>30</sup> |                     | 1.00 <sup>40</sup> |                      | 0.344 <sup>30</sup> (Ne); 0.189 <sup>40</sup> (Ar);<br>13.6 <sup>50</sup> (propyne)                                                                                         |
| Poly(acrylonitrile)    |                     |                       |                    | 0.000 2             | 0.000 8            | 300                  |                                                                                                                                                                             |

**TABLE 10.5** Gas Permeability Constants ( $10^{10} P$ ) at 25°C for Polymers and Rubbers (*Continued*)

| Polymer or rubber                           | Gas  |                |                    |                |                 |                   |                                                                                                                                                                                                                                                                |
|---------------------------------------------|------|----------------|--------------------|----------------|-----------------|-------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                             | He   | N <sub>2</sub> | H <sub>2</sub>     | O <sub>2</sub> | CO <sub>2</sub> | H <sub>2</sub> O  | Other                                                                                                                                                                                                                                                          |
| Acrylonitrile-styrene copolymer (66 : 34)   |      |                |                    | 0.048          | 0.21            | 2 000             |                                                                                                                                                                                                                                                                |
| Poly(1,3-butadiene)                         |      | 6.42           | 41.9               | 19.0           | 138.0           | 5 070             |                                                                                                                                                                                                                                                                |
| Poly ( <i>cis</i> -1,4-butadiene)           | 32.6 | 19.2           |                    |                |                 |                   | 19.2 (Ne); 41.0 (Ar)                                                                                                                                                                                                                                           |
| Butadiene-acrylonitrile copolymer (80 : 20) | 12.2 | 1.06           | 15.9               | 3.85           | 30.8            |                   | 24.8 (C <sub>2</sub> H <sub>2</sub> ); 7.7 (propyne)                                                                                                                                                                                                           |
| Butadiene-styrene copolymer (80 : 20)       | 13.4 | 1.71           |                    |                |                 |                   | 5.01 (Ne); 4.49 (Ar)                                                                                                                                                                                                                                           |
| Butadiene-styrene copolymer (92 : 8)        | 22.9 | 5.11           |                    |                |                 |                   | 9.70 (Ne); 12.7 (Ar)                                                                                                                                                                                                                                           |
| Polychloroprene                             |      | 1.2            | 13.6               | 4.0            | 25.8            |                   | 3.79 (Ar); 3.27 (CH <sub>4</sub> )                                                                                                                                                                                                                             |
| Polyethylene, low-density                   | 4.9  | 0.969          | 12.0 <sup>30</sup> | 2.88           | 12.6            | 90                | 2.88 (CH <sub>4</sub> ); 6.81 (C <sub>2</sub> H <sub>6</sub> );<br>9.43 (C <sub>3</sub> H <sub>8</sub> ); 1.48 CO;<br>49 <sup>0</sup> (ethylene oxide);<br>14.4 (propene); 42.2 (propyne);<br>0.170 (SF <sub>6</sub> ); 472 <sup>60</sup> (CH <sub>3</sub> Br) |
| Polyethylene, high-density                  | 1.14 | 0.143          | 3.0 <sup>20</sup>  | 0.403          | 0.36            | 12.0              | 0.388 (CH <sub>4</sub> ); 0.590 (C <sub>2</sub> H <sub>6</sub> );<br>0.537 (C <sub>3</sub> H <sub>8</sub> ); 0.008 3 (SF <sub>6</sub> );<br>1.69 (Ar); 4.01 (propene)                                                                                          |
| Poly(ethylene terephthalate)                |      |                |                    |                |                 |                   |                                                                                                                                                                                                                                                                |
| Crystalline                                 | 1.32 | 0.006 5        | 3.70 <sup>20</sup> | 0.035          | 0.17            | 130               | 0.003 2 (CH <sub>4</sub> ); 0.08 <sup>60</sup> (CH <sub>3</sub> Br)                                                                                                                                                                                            |
| Amorphous                                   | 3.28 | 0.013          |                    | 0.059          | 0.30            |                   | 0.009 (CH <sub>4</sub> )                                                                                                                                                                                                                                       |
| Poly(ethyl methacrylate)                    | 6.82 | 0.220          |                    | 1.15           | 5.00            | 3 200             | 2.98 (Ne); 0.565 (Ar); 0.370 (Kr);<br>3.83 (H <sub>2</sub> S); 0.000 001 65 (SF <sub>6</sub> )                                                                                                                                                                 |
| Isobutene-isoprene copolymer (98 : 2)       | 8.38 | 0.324          | 7.20               | 1.30           | 5.16            | 110 <sup>38</sup> | 13.6 <sup>50</sup> (C <sub>3</sub> H <sub>8</sub> )                                                                                                                                                                                                            |
| Isoprene-acrylonitrile copolymer (76 : 24)  | 7.77 | 0.181          | 7.41               | 0.852          | 4.32            |                   |                                                                                                                                                                                                                                                                |

**TABLE 10.5** Gas Permeability Constants ( $10^{10} P$ ) at 25°C for Polymers and Rubbers (*Continued*)

| Polymer or rubber                                      | Gas                 |                        |                    |                       |                     |                      |                                                                                                                                    |
|--------------------------------------------------------|---------------------|------------------------|--------------------|-----------------------|---------------------|----------------------|------------------------------------------------------------------------------------------------------------------------------------|
|                                                        | He                  | N <sub>2</sub>         | H <sub>2</sub>     | O <sub>2</sub>        | CO <sub>2</sub>     | H <sub>2</sub> O     | Other                                                                                                                              |
| Isoprene-methacrylonitrile copolymer (76:24)           |                     | 0.596                  | 13.6               | 2.34                  | 14.1                |                      |                                                                                                                                    |
| Methacrylonitrile-styrene-butadiene copolymer (88:7:5) |                     |                        |                    | 0.004 8               | 0.014               | 600                  |                                                                                                                                    |
| Poly(methylpentene)                                    | 101                 | 7.83                   | 136                | 32.0                  | 92.6                |                      |                                                                                                                                    |
| Polypropylene                                          | 38 <sup>20</sup>    | 0.44 <sup>30</sup>     | 41 <sup>20</sup>   | 2.3 <sup>30</sup>     | 9.2 <sup>30</sup>   | 51                   | 0.33 <sup>20</sup> (H <sub>2</sub> S); 9.2 <sup>20</sup> (NH <sub>3</sub> )                                                        |
| Silicone rubber, 10% filler                            | 233 <sup>0</sup>    | 227 <sup>0</sup>       | 464 <sup>0</sup>   | 489 <sup>0</sup>      | 3 240               | 43 000 <sup>35</sup> | 191 <sup>0</sup> (Ne); 550 <sup>0</sup> (Ar);<br>1 020 <sup>0</sup> (Kr); 2 550 <sup>0</sup> (Xe);<br>19 000 <sup>0</sup> (butane) |
| Polystyrene                                            | 18.7                | 0.788                  | 23.3               | 2.63                  | 10.5                | 1 200                |                                                                                                                                    |
| Poly(tetrafluoroethylene)                              |                     | 1.4                    | 9.8                | 4.2                   | 11.7                |                      | 15.7 (NO <sub>2</sub> ); 37.5 (N <sub>2</sub> O <sub>4</sub> )                                                                     |
| Poly(trifluoroethylene)                                | 6.8 <sup>20</sup>   | 0.003                  | 0.94 <sup>20</sup> | 0.025 <sup>40</sup>   | 0.048 <sup>40</sup> | 0.29                 | 1.2 <sup>0</sup> (ethylene oxide);<br>4.6 <sup>60</sup> (CH <sub>3</sub> Br)                                                       |
| Poly(vinyl acetate)                                    | 12.6 <sup>30</sup>  |                        | 89 <sup>30</sup>   | 0.50 <sup>30</sup>    |                     |                      | 2.64 <sup>30</sup> (Ne); 0.19 <sup>30</sup> (Ar);<br>0.078 <sup>30</sup> (Kr); 0.050 <sup>30</sup> (CH <sub>4</sub> )              |
| Poly(vinyl alcohol)                                    | 0.001 <sup>30</sup> | <0.001 <sup>14</sup>   | 0.009              | 0.008 9               | 0.001 <sup>23</sup> |                      | 0.007 (H <sub>2</sub> S); 0.002 <sup>0</sup><br>(ethylene oxide)                                                                   |
| Poly(vinyl chloride)                                   | 2.05                | 0.011 8                | 1.70               | 0.045 3               | 0.157               | 275                  | 3.92 (Ne); 0.011 5 (Ar);<br>0.028 6 (CH <sub>4</sub> )                                                                             |
| Poly(vinylidene chloride)                              | 0.31 <sup>34</sup>  | 0.000 94 <sup>30</sup> |                    | 0.005 3 <sup>30</sup> | 0.03 <sup>30</sup>  | 0.5                  | 0.03 <sup>30</sup> (H <sub>2</sub> S); 0.008 <sup>60</sup> (CH <sub>3</sub> Br)                                                    |

**TABLE 10.6** Vapor Permeability Constants ( $10^{10} P$ ) at 35°C for Polymers  
*All tabulated values are multiplied by  $10^{10}$  and are in units of  $\text{seconds}^{-1}$  (centimeters of Hg) $^{-1}$ .*

| Polymer                   | Vapor   |        |                      |         |               |
|---------------------------|---------|--------|----------------------|---------|---------------|
|                           | Benzene | Hexane | Carbon tetrachloride | Ethanol | Ethyl acetate |
| Cellulose                 | 1.4     | 0.912  | 0.836                | 85.8    | 13.4          |
| Cellulose acetate         | 512     | 2.80   | 3.74                 | 2 980   | 3 595         |
| Poly(acrylonitrile)       | 2.61    | 1.59   | 1.47                 | 0       | 1.34          |
| Polyethylene, low-density | 5 300   | 2 910  | 3 810                | 55.9    | 513           |
| Polystyrene               | 10 600  |        | 6 820                | 0       | soluble       |
| Poly(vinyl alcohol)       | 3.58    | 2.34   | 1.61                 | 32.7    | 2.53          |

### 10.7 FATS, OILS, AND WAXES

**TABLE 10.7** Constants of Fats and Oils

| Fat or oil    | Solidification point, °C | Specific gravity (15°C/15°C)         | Refractive index      | Acid value | Saponification value | Iodine value |
|---------------|--------------------------|--------------------------------------|-----------------------|------------|----------------------|--------------|
| Animal origin |                          |                                      |                       |            |                      |              |
| Butterfat     | 20–23                    | 0.91 <sup>40°C</sup> <sub>15°C</sub> | 1.45 <sup>40°C</sup>  | 0.5–35     | 210–230              | 26–38        |
| Chicken fat   | 21–27                    | 0.924                                |                       | 1.2        | 193–205              | 66–72        |
| Cod-liver oil | –3                       | 0.92–0.93                            | 1.481 <sup>25°C</sup> | 5.6        | 171–189              | 137–166      |
| Deer fat      |                          | 0.96–0.97                            |                       | 0.8–5.3    | 195–200              | 26–36        |

**TABLE 10.7** Constants of Fats and Oils (*Continued*)

| Fat or oil                         | Solidification point, °C | Specific gravity (15°C/15°C)      | Refractive index       | Acid value | Saponification value     | Iodine value            |
|------------------------------------|--------------------------|-----------------------------------|------------------------|------------|--------------------------|-------------------------|
| Animal origin ( <i>continued</i> ) |                          |                                   |                        |            |                          |                         |
| Dolphin                            | − 3 to + 5               | 0.91–0.93                         |                        | 2–12       | 203 (body);<br>290 (jaw) | 127 (body);<br>33 (jaw) |
| Goat butter                        |                          | 0.91–0.94 <sup>38°C</sup><br>38°C |                        |            | 233–236                  | 25–37                   |
| Goose fat                          | 22–24                    | 0.92–0.93                         |                        | 0.6        | 191–193                  | 58–67                   |
| Herring oil                        |                          | 0.92–0.94                         | 1.4610 <sup>60°C</sup> | 1.8–44     | 170–194                  | 102–149                 |
| Horse fat                          | 20–45                    | 0.92–0.93                         |                        | 0–2.4      | 195–200                  | 75–86                   |
| Human fat                          | 15                       | 0.903                             | 1.460                  |            | 193–200                  | 57–73                   |
| Lard oil                           | − 2 to + 4               | 0.913–0.915                       | 1.462                  | 0.1–2.5    | 193–198                  | 63–79                   |
| Lard oil, fatty tissue             | 27–30                    | 0.93–0.94                         | 1.462                  | 0.5–0.8    | 195–203                  | 47–67                   |
| Menhaden oil                       | − 5                      | 0.92–0.93                         | 1.465 <sup>60°C</sup>  | 3–12       | 189–193                  | 148–185                 |
| Neat’s-foot oil                    | − 2 to + 10              | 0.91–0.92                         | 1.464 <sup>25°C</sup>  | 0.1–0.6    | 193–199                  | 58–75                   |
| Porpoise, body oil                 | − 16                     | 0.926                             |                        | 1.2        | 203                      | 127                     |
| Rabbit fat                         | 17–23                    | 0.93–0.94                         |                        | 1.4–7.2    | 199–203                  | 70–100                  |
| Sardine oil                        | 20–22                    | 0.92–0.93                         | 1.466 <sup>60°C</sup>  | 4–25       | 188–196                  | 130–152                 |
| Seal                               | 3                        | 0.915–0.926                       |                        | 1.9–40     | 188–196                  | 130–152                 |
| Shark                              |                          | 0.916–0.919                       |                        |            | 157–164                  | 115–139                 |
| Sperm oil                          | 15.5                     | 0.878–0.884                       |                        | 13         | 120–137                  | 80–84                   |
| Tallow, beef                       | 31–38                    | 0.895                             |                        | 0.25       | 196–200                  | 35–42                   |
| Tallow, mutton                     | 32–41                    | 0.937–0.953                       | 1.457 <sup>40°C</sup>  | 2–14       | 195–196                  | 48–61                   |
| Whale oil                          | − 2 to 0                 | 0.917–0.924                       | 1.460 <sup>60°C</sup>  | 1.9        | 160–202                  | 90–146                  |
| Plant origin                       |                          |                                   |                        |            |                          |                         |
| Acorn                              | − 10                     | 0.916                             |                        |            | 199                      | 100                     |
| Almond                             | − 20 to − 15             | 0.914–0.921                       |                        | 0.5–3.5    | 183–208                  | 93–103                  |
| Babassu oil                        | 22–26                    | 0.893 <sup>60°C</sup>             | 1.443 <sup>60°C</sup>  |            | 247                      | 16                      |
| Beechnut oil                       | − 17                     | 0.922                             |                        |            | 191–196                  | 97–111                  |



**TABLE 10.7** Constants of Fats and Oils (*Continued*)

| Fat or oil                        | Solidification point, °C | Specific gravity (15°C/15°C)          | Refractive index      | Acid value | Saponification value | Iodine value |
|-----------------------------------|--------------------------|---------------------------------------|-----------------------|------------|----------------------|--------------|
| Plant origin ( <i>continued</i> ) |                          |                                       |                       |            |                      |              |
| Castor oil                        | − 18 to − 17             | 0.960–0.967                           | 1.477                 | 0.1–0.8    | 175–183              | 84           |
| Chaulmoogra oil, USP              | < − 25                   | 0.950 <sup>25°C</sup>                 |                       |            | 196–213              | 98–110       |
| Chinese vegetable tallow          | 24–34                    | 0.918–0.922                           |                       | 2.4        | 179–206              | 23–41        |
| Cocoa butter                      | 21.5–23                  | 0.964–0.974                           | 1.457 <sup>40°C</sup> | 1.1–1.9    | 193–195              | 33–42        |
| Coconut oil                       | 14–22                    | 0.926                                 | 1.449 <sup>40°C</sup> | 2.5–10     | 153–262              | 6–10         |
| Corn (maize) oil                  | − 20 to − 10             | 0.921–0.928                           | 1.473 <sup>40°C</sup> | 1.4–2.0    | 187–193              | 111–128      |
| Cottonseed oil                    | − 13 to + 12             | 0.918 <sup>25°C</sup> <sub>25°C</sub> | 1.474 <sup>40°C</sup> | 0.6–0.9    | 194–196              | 103–111      |
| Hazelnut oil                      | − 18 to − 17             | 0.917                                 |                       |            | 191–197              | 87           |
| Hemp-seed oil                     | − 28 to − 15             | 0.928–0.934                           |                       | 0.45       | 190–195              | 145–162      |
| Linseed oil                       | − 27 to − 19             | 0.930–0.938                           | 1.478 <sup>25°C</sup> | 1–3.5      | 188–195              | 175–202      |
| Mustard, black, oil               | 16                       | 0.918–0.921                           | 1.475 <sup>40°C</sup> | 5.7–7.3    | 173–175              | 99–110       |
| Neem oil                          | − 3                      | 0.917                                 | 1.462 <sup>40°C</sup> |            | 195                  | 71           |
| Niger-seed oil                    |                          | 0.925                                 | 1.471 <sup>40°C</sup> |            | 190                  | 129          |
| Oiticica oil                      |                          | 0.974 <sup>25°C</sup>                 |                       |            |                      | 140–180      |
| Olive oil                         | − 6                      | 0.914–0.918                           | 1.468 <sup>40°C</sup> | 0.3–1.0    | 185–196              | 79–88        |
| Palm oil                          | 35–42                    | 0.915                                 | 1.458 <sup>40°C</sup> | 10         | 200–205              | 49–59        |
| Palm kernel oil                   | 24                       | 0.918–0.925                           | 1.457 <sup>40°C</sup> | 0.3–0.6    | 220–231              | 26–32        |
| Peanut oil                        | 3                        | 0.917–0.926                           | 1.469 <sup>40°C</sup> | 0.8        | 186–194              | 88–98        |
| Perilla oil                       |                          | 0.930–0.937                           | 1.481 <sup>25°C</sup> |            | 188–194              | 185–206      |
| Pistachio-nut oil                 | − 10 to − 5              | 0.913–0.919                           |                       |            | 191                  | 83–87        |
| Poppy-seed oil                    | − 18 to − 16             | 0.924–0.926                           | 1.469 <sup>40°C</sup> | 2.5        | 193–195              | 128–141      |
| Pumpkin-seed oil                  | − 15                     | 0.923–0.925                           |                       |            | 188–193              | 121–130      |
| Rapeseed oil                      | − 10                     | 0.913–0.917                           | 1.471 <sup>40°C</sup> | 0.36–1.0   | 168–179              | 94–105       |
| Safflower oil                     | − 18 to − 13             | 0.925–0.928                           | 1.462 <sup>60°C</sup> | 0.6        | 188–203              | 122–141      |
| Sesame oil                        | − 6 to − 4               | 0.919 <sup>25°C</sup> <sub>25°C</sub> | 1.465 <sup>40°C</sup> | 9.8        | 188–193              | 103–117      |
| Soybean oil                       | − 16 to − 10             | 0.924–0.927                           | 1.473 <sup>40°C</sup> | 0.3–1.8    | 189–194              | 122–134      |
| Sunflower-seed oil                | − 17                     | 0.924–0.926                           | 1.469 <sup>40°C</sup> | 11.2       | 188–193              | 129–136      |
| Tung oil                          | − 2.5                    | 0.94–0.95                             | 1.517 <sup>25°C</sup> | 2          | 190–197              | 163–171      |
| White-mustard-seed oil            | − 16 to − 8              | 0.912–0.916                           |                       | 5.4        | 171–174              | 94–98        |
| Wheat-germ oil                    |                          |                                       |                       |            |                      | 125          |

**TABLE 10.8** Constants of Waxes

| Wax                      | Melting point, °C | Specific gravity (15°C/15°C) | Refractive index          | Acid value | Saponification value | Iodine value |
|--------------------------|-------------------|------------------------------|---------------------------|------------|----------------------|--------------|
| Bamboo leaf              | 79–80             | 0.961 <sup>25°C</sup>        |                           | 14–15      | 43–44                | 7.8          |
| Bayberry (myrtle)        | 47–49             | 0.99                         | 1.436 <sup>90°C</sup>     | 3–4        | 205–212              | 4–9.5        |
| Beeswax, ordinary        | 62–66             | 0.95–0.97                    | 1.44–1.48 <sup>40°C</sup> | 17–21      | 88–100               | 8–11         |
| Beeswax, East Indian     | 61–67             | 0.95–0.97                    | 1.44 <sup>40°C</sup>      | 5–10.5     | 87–117               | 4–10.5       |
| Beeswax, white, USP      | 61–69             | 0.95–0.98                    | 1.45–1.47 <sup>65°C</sup> | 17–24      | 90–96                | 7–11         |
| Candelilla               | 73–77             | 0.98–0.99                    | 1.45–1.46 <sup>85°C</sup> | 19–24      | 55–64                | 14–20        |
| Cape berry               | 40–45             | 1.01                         | 1.45 <sup>45°C</sup>      | 2.5–4.0    | 211–215              | 0.5–2.5      |
| Caranda                  | 80–85             | 0.99–1.00                    |                           | 5.0–9.5    | 64–79                | 8–9          |
| Carnauba, No. 1 yellow   | 86–88             | 0.99–1.00                    |                           | 1.5–2.5    | 75–86                |              |
| Carnauba, No. 3, crude   | 86–90             | 0.99–1.01                    |                           | 3.0–8.5    | 75–89                |              |
| Carnauba, No. 3, refined | 86–89             | 0.96–0.97                    | 1.47 <sup>40°C</sup>      | 3.0–5.0    | 76–85                | 7–13.5       |
| Castor oil, hydrogenated | 83–88             | 0.98–0.99 <sup>20°C</sup>    |                           | 1.0–5.0    | 177–181              | 2.5–8.5      |
| Chinese insect           | 80–85             | 0.95–0.97                    | 1.46 <sup>40°C</sup>      | 2–9        | 78–93                | 1.0–2.5      |
| Cotton                   | 68–71             | 0.96                         |                           | 32         | 71                   | 25           |
| Cranberry                | 207–218           | 0.97–0.98                    |                           | 42–59      | 131–134              | 44–53        |
| Esparto                  | 75–79             | 0.985–0.995                  |                           | 22–27      | 58–73                | 7–15         |
| Flax                     | 61–70             | 0.91–0–0.99                  |                           | 17–48      | 37–102               | 22–29        |
| Japan                    | 49–56             | 0.97–1.00                    |                           | 4–15       | 210–235              | 4–15         |
| Jojoba                   | 11–12             | 0.86–0.90 <sup>25°C</sup>    | 1.465 <sup>25°C</sup>     | 0.2–0.6    | 92–95                | 82–88        |

**TABLE 10.8** Constants of Waxes (Continued)

| Wax                     | Melting<br>point, °C | Specific<br>gravity<br>(15°C/15°C) | Refractive<br>index       | Acid<br>value | Saponification<br>value | Iodine<br>value |
|-------------------------|----------------------|------------------------------------|---------------------------|---------------|-------------------------|-----------------|
| Microcrystalline, amber | 64–91                | 0.91–0.94                          | 1.42–1.45 <sup>80°C</sup> | 0             | 0                       | 0               |
| Microcrystalline, white | 71–89                | 0.93–0.94                          | 1.441 <sup>80°C</sup>     | 0             | 0                       | 0               |
| Montan, crude           | 76–86                | 1.01–1.02 <sup>25°C</sup>          |                           | 22–31         | 59–92                   | 14–18           |
| Montan, refined         | 77–84                | 1.02–1.04                          |                           | 23–45         | 72–115                  | 10–14           |
| Ouricury                | 86–89                | 0.99–1.01                          |                           | 12–19         | 88–96                   | 6.9–7.8         |
| Ozokerite               | 56–82                | 0.90–1.00                          |                           | 0             | 0                       | 4–8             |
| Palm                    | 74–86                | 0.99–1.05                          |                           | 5–11          | 64–104                  | 9–17            |
| Paraffin, American      | 49–63                | 0.896–0.925                        | 1.44–1.48 <sup>80°C</sup> | 0             | 0                       | 0               |
| Shellac                 | 79–82                | 0.97–0.98                          |                           | 12–24         | 64–83                   | 6–9             |
| Sisal hemp              | 74–81                | 1.007–1.010                        |                           | 16–19         | 56–58                   | 28–29           |
| Spermaceti              | 41–49                | 0.905–0.960                        |                           | 0.5–3.0       | 121–135                 | 2.5–8.5         |
| Sugarcane, refined      | 76–82                | 0.96–0.98                          | 1.51 <sup>25°C</sup>      | 8–23          | 55–70                   | 13–29           |
| Wool                    | 38–40                | 0.97                               | 1.48 <sup>40°C</sup>      | 6–22          | 82–130                  | 15–47           |

---

# SECTION 11

---

## PRACTICAL LABORATORY INFORMATION

---

|                                                                                                                                                                                      |              |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|
| <b>11.1 COOLING</b>                                                                                                                                                                  | <b>11.3</b>  |
| Table 11.1 Cooling Mixtures                                                                                                                                                          | 11.3         |
| Table 11.2 Molecular Lowering of the Melting or Freezing Point                                                                                                                       | 11.4         |
| <b>11.2 DRYING AND HUMIDIFICATION</b>                                                                                                                                                | <b>11.5</b>  |
| Table 11.3 Drying Agents                                                                                                                                                             | 11.5         |
| Table 11.4 Solutions for Maintaining Constant Humidity                                                                                                                               | 11.6         |
| Table 11.5 Concentration of Solutions of $\text{H}_2\text{SO}_4$ , $\text{NaOH}$ , and $\text{CaCl}_2$ Giving Specified Vapor Pressures and Percent Humidities at $25^\circ\text{C}$ | 11.7         |
| Table 11.6 Relative Humidity from Wet and Dry Bulb Thermometer Readings                                                                                                              | 11.8         |
| Table 11.7 Relative Humidity from Dew Point Readings                                                                                                                                 | 11.9         |
| <b>11.3 BOILING POINTS AND HEATING BATHS</b>                                                                                                                                         | <b>11.10</b> |
| Table 11.8 Organic Solvents Arranged by Boiling Points                                                                                                                               | 11.10        |
| Table 11.9 Molecular Elevation of the Boiling Point                                                                                                                                  | 11.13        |
| Table 11.10 Substances Which Can Be Used for Heating Baths                                                                                                                           | 11.15        |
| <b>11.4 SEPARATION METHODS</b>                                                                                                                                                       | <b>11.16</b> |
| Table 11.11 Solvents of Chromatographic Interest                                                                                                                                     | 11.16        |
| Table 11.12 Solvents Having the Same Refractive Index and the Same Density at $25^\circ\text{C}$                                                                                     | 11.18        |
| Table 11.13 McReynolds' Constants for Stationary Phases in Gas Chromatography                                                                                                        | 11.21        |
| <b>11.4.1 McReynolds' Constants</b>                                                                                                                                                  | <b>11.26</b> |
| Table 11.14 Characteristics of Selected Supercritical Fluids                                                                                                                         | 11.26        |
| <b>11.4.2 Chromatographic Behavior of Solutes</b>                                                                                                                                    | <b>11.27</b> |
| Table 11.15 Typical Performances in HPLC for Various Conditions                                                                                                                      | 11.31        |
| <b>11.4.3 Ion-Exchange (Normal Pressure, Columnar)</b>                                                                                                                               | <b>11.32</b> |
| Table 11.16 Guide to Ion-Exchange Resins                                                                                                                                             | 11.33        |
| Table 11.17 Relative Selectivity of Various Counter Cations                                                                                                                          | 11.37        |
| Table 11.18 Relative Selectivity of Various Counter Anions                                                                                                                           | 11.38        |
| <b>11.5 GRAVIMETRIC ANALYSIS</b>                                                                                                                                                     | <b>11.41</b> |
| Table 11.19 Gravimetric Factors                                                                                                                                                      | 11.41        |
| Table 11.20 Elements Precipitated by General Analytical Reagents                                                                                                                     | 11.67        |
| Table 11.21 Cleaning Solutions for Fritted Glassware                                                                                                                                 | 11.69        |
| Table 11.22 Common Fluxes                                                                                                                                                            | 11.70        |
| Table 11.23 Membrane Filters                                                                                                                                                         | 11.70        |
| Table 11.24 Porosities of Fritted Glassware                                                                                                                                          | 11.71        |
| Table 11.25 Tolerances for Analytical Weights                                                                                                                                        | 11.71        |
| Table 11.26 Heating Temperatures, Composition of Weighing Forms, and Gravimetric Factors                                                                                             | 11.72        |
| <b>11.6 VOLUMETRIC ANALYSIS</b>                                                                                                                                                      | <b>11.74</b> |
| <b>11.6.1 Acid-Base Titrations in Aqueous Media</b>                                                                                                                                  | <b>11.74</b> |
| Table 11.27 Primary Standards for Aqueous Acid-Base Titrations                                                                                                                       | 11.74        |
| Table 11.28 Titrimetric (Volumetric) Factors                                                                                                                                         | 11.76        |
| <b>11.6.2 Titrimetric (Volumetric) Factors for Acid-Base Titrations</b>                                                                                                              | <b>11.82</b> |
| <b>11.6.3 Standard Volumetric (Titrimetric) Redox Solutions</b>                                                                                                                      | <b>11.82</b> |
| <b>11.6.4 Indicators for Redox Titrations</b>                                                                                                                                        | <b>11.83</b> |
| Table 11.29 Equations for the Redox Determinations of the Elements with Equivalent Weights                                                                                           | 11.84        |

|             |                                                                                                             |        |
|-------------|-------------------------------------------------------------------------------------------------------------|--------|
| 11.6.5      | Precipitation Titrations                                                                                    | 11.89  |
| 11.6.6      | Complexometric Titrations                                                                                   | 11.89  |
| 11.6.7      | Masking Agents                                                                                              | 11.92  |
| 11.6.8      | Demasking                                                                                                   | 11.93  |
| Table 11.30 | Standard Solutions for Precipitation Titrations                                                             | 11.94  |
| Table 11.31 | Indicators for Precipitation Titrations                                                                     | 11.95  |
| Table 11.32 | Properties and Applications of Selected Metal Ion Indicators                                                | 11.96  |
| Table 11.33 | Variation of $\alpha_4$ with pH                                                                             | 11.97  |
| Table 11.34 | Formation Constants of EDTA Complexes at 25°C, Ionic Strength Approaching Zero                              | 11.97  |
| Table 11.35 | Cumulative Formation Constants of Ammine Complexes at 20°C, Ionic Strength 0.1                              | 11.97  |
| Table 11.36 | Masking Agents for Various Elements                                                                         | 11.98  |
| Table 11.37 | Masking Agents for Anions and Neutral Molecules                                                             | 11.100 |
| Table 11.38 | Common Demasking Agents                                                                                     | 11.100 |
| Table 11.39 | Amino Acids $pI$ and $pK_a$ Values                                                                          | 11.102 |
| Table 11.40 | Tolerances of Volumetric Flasks                                                                             | 11.102 |
| Table 11.41 | Pipet Capacity Tolerances                                                                                   | 11.103 |
| Table 11.42 | Tolerances of Micropipets (Eppendorf)                                                                       | 11.103 |
| Table 11.43 | Buret Accuracy Tolerances                                                                                   | 11.103 |
| Table 11.44 | Factors for Simplified Computation of Volume                                                                | 11.104 |
| Table 11.45 | Cubical Coefficients of Thermal Expansion                                                                   | 11.105 |
| Table 11.46 | General Solubility Rules for Inorganic Compounds                                                            | 11.105 |
| 11.7        | LABORATORY SOLUTIONS                                                                                        | 11.106 |
| Table 11.47 | Concentration of Commonly Used Acids and Bases                                                              | 11.106 |
| Table 11.48 | Standard Stock Solutions                                                                                    | 11.107 |
| 11.7.1      | General Reagents, Indicators, and Special Solutions                                                         | 11.109 |
| Table 11.49 | TLV Concentration Limits for Gases and Vapors                                                               | 11.121 |
| Table 11.50 | Some Common Reactive and Incompatible Chemicals                                                             | 11.130 |
| Table 11.51 | Chemicals Recommended for Refrigerated Storage                                                              | 11.136 |
| Table 11.52 | Chemicals Which Polymerize or Decompose on Extended Refrigeration                                           | 11.136 |
| 11.8        | SIEVES AND SCREENS                                                                                          | 11.137 |
| Table 11.53 | U.S. Standard Sieve Series                                                                                  | 11.137 |
| 11.9        | THERMOMETRY                                                                                                 | 11.137 |
| 11.9.1      | Temperature and Its Measurement                                                                             | 11.137 |
| Table 11.54 | Fixed Points in the ITS-90                                                                                  | 11.138 |
| 11.10       | THERMOCOUPLES                                                                                               | 11.138 |
| Table 11.55 | Thermoelectric Values in Millivolts at Fixed Points for Various Thermocouples                               | 11.140 |
| Table 11.56 | Type B Thermocouples: Platinum–30% Rhodium Alloy vs. Platinum–6% Rhodium Alloy                              | 11.142 |
| Table 11.57 | Type E Thermocouples: Nickel-Chromium Alloy vs. Copper-Nickel Alloy                                         | 11.143 |
| Table 11.58 | Type J Thermocouples: Iron vs. Copper-Nickel Alloy                                                          | 11.144 |
| Table 11.59 | Type K Thermocouples: Nickel-Chromium Alloy vs. Nickel-Aluminum Alloy                                       | 11.145 |
| Table 11.60 | Type N Thermocouples: Nickel–14.2% Chromium–1.4% Silicon Alloy vs. Nickel–4.4% Silicon–0.1% Magnesium Alloy | 11.146 |
| Table 11.61 | Type R Thermocouples: Platinum–13% Rhodium Alloy vs. Platinum                                               | 11.147 |
| Table 11.62 | Type S Thermocouples: Platinum–10% Rhodium Alloy vs. Platinum                                               | 11.148 |
| Table 11.63 | Type T Thermocouples: Copper vs. Copper-Nickel Alloy                                                        | 11.149 |
| 11.11       | CORRECTION FOR EMERGENT STEM OF THERMOMETERS                                                                | 11.150 |
| Table 11.64 | Values of $K$ for Stem Correction of Thermometers                                                           | 11.150 |

## 11.1 COOLING

**TABLE 11.1** Cooling Mixtures

The table below gives the lowest temperature that can be obtained from a mixture of the inorganic salt with finely shaved dry ice. With the organic substances, dry ice ( $-78^{\circ}\text{C}$ ) in small lumps can be added to the solvent until a slight excess of dry ice remains or liquid nitrogen ( $-196^{\circ}\text{C}$ ) can be poured into the solvent until a slush is formed that consists of the solid-liquid mixture at its melting point.

| Substance                  | Quantity of substance, g | Quantity of water, mL | Temperature, $^{\circ}\text{C}$ |
|----------------------------|--------------------------|-----------------------|---------------------------------|
| Ammonium nitrate           | 100                      | 94                    | $-4.0$                          |
| Sodium nitrate             | 75                       | 100                   | $-5.3$                          |
| Sodium thiosulfate 5-water | 110                      | 100                   | $-8.0$                          |
| Sodium chloride            | 36                       | 100                   | $-10.0$                         |
| Sodium nitrate             | 50                       | 100                   | $-17.8$                         |
| Sodium bromide             | 66                       | 100                   | $-28$                           |
| Magnesium chloride         | 85                       | 100                   | $-34$                           |
| Calcium chloride 6-water   | 100                      | 81                    | $-40.3$                         |
|                            | 100                      | 70                    | $-55$                           |

| Substance                | Temperature, $^{\circ}\text{C}$ | Substance        | Temperature, $^{\circ}\text{C}$ |
|--------------------------|---------------------------------|------------------|---------------------------------|
| Ethylene glycol          | $-13$                           | Acetone          | $-77$                           |
| 1,2-Dichlorobenzene      | $-17$                           | Ethyl acetate    | $-84$                           |
| Carbon tetrachloride     | $-22.9$                         | 2-Butanone       | $-87$                           |
| Bromobenzene             | $-31$                           | Hexane           | $-95$                           |
| Methoxybenzene           | $-37$                           | Methanol         | $-98$                           |
| Bis(2-ethoxyethyl) ether | $-44$                           | Carbon disulfide | $-112$                          |
| Chlorobenzene            | $-45$                           | Bromoethane      | $-119$                          |
| <i>N</i> -Methylaniline  | $-57$                           | Pentane          | $-130$                          |
| <i>p</i> -Cymene         | $-68$                           | 2-Methylbutane   | $-160$                          |

**TABLE 11.2** Molecular Lowering of the Melting or Freezing Point  
*Cryoscopic constants.*

The cryoscopic constant  $K_f$  gives the depression of the melting point  $\Delta T$  (in degrees Celsius) produced when 1 mol of solute is dissolved in 1000 g of a solvent. It is applicable only to dilute solutions for which the number of moles of solute is negligible in comparison with the number of moles of solvent. It is often used for molecular weight determinations.

$$M_2 = \frac{1000w_2K_f}{w_1 \Delta T}$$

where  $w_1$  is the weight of the solvent and  $w_2$  is the weight of the solute whose molecular weight is  $M_2$ .

| Compound                           | $K_f$ | Compound                                        | $K_f$      |
|------------------------------------|-------|-------------------------------------------------|------------|
| Acetamide                          | 4.04  | Diphenylamine                                   | 8.60       |
| Acetic acid                        | 3.90  | Diphenyl ether                                  | 7.88       |
| Acetone                            | 2.40  | 1,2-Ethanediamine                               | 2.43       |
| Ammonia                            | 0.957 | Ethoxybenzene                                   | 7.15       |
| Aniline                            | 5.87  | Formamide                                       | 3.85       |
| Antimony(III) chloride             | 17.95 | Formic acid                                     | 2.77       |
| Benzene                            | 5.12  | Glycerol                                        | 3.3 to 3.7 |
| Benzonitrile                       | 5.34  | Hexamethylphosphoramide                         | 6.93       |
| Benzophenone                       | 9.8   |                                                 |            |
| Bicyclohexane                      | 14.52 | <i>N</i> -Methylacetamide                       | 6.65       |
| Biphenyl                           | 8.0   | 2-Methyl-2-butanol                              | 10.4       |
| Borneol                            | 35.8  | Methylcyclohexane                               | 14.13      |
| Bornylamine                        | 40.6  | Methyl <i>cis</i> -9-octadecenoate              | 3.4        |
| Butanedinitrile                    | 18.26 | 2-Methyl-2-propanol                             | 8.37       |
| Camphene                           | 31.08 | Naphthalene                                     | 6.94       |
| Camphoquinone                      | 45.7  | Nitrobenzene                                    | 6.852      |
| <b>D</b> -(+)-Camphor              | 39.7  | Octadecanoic acid                               | 4.50       |
| Carbon tetrachloride               | 29.8  | 2-Oxohexamethyleneimine                         | 7.30       |
| <i>o</i> -Cresol                   | 5.60  | Phenol                                          | 7.40       |
| <i>p</i> -Cresol                   | 6.96  | Pyridine                                        | 4.75       |
| Cyclohexane                        | 20.0  | Quinoline                                       | 1.95       |
| Cyclohexanol                       | 39.3  | Succinonitrile                                  | 18.26      |
| Cyclohexylcyclohexane              | 14.52 | Sulfuric acid                                   | 1.86       |
| Cyclopentadecanone                 | 21.3  | 1,1,2,2-Tetrabromoethane                        | 21.7       |
| <i>cis</i> -Decahydronaphthalene   | 19.47 | 1,1,2,2-Tetrachloro-<br>1,2-difluoroethane      | 37.7       |
| <i>trans</i> -Decahydronaphthalene | 20.81 | Tetramethylene sulfone                          | 64.1       |
| Dibenz[ <i>de,kl</i> ]anthracene   | 25.7  | <i>p</i> -Toluidine                             | 5.372      |
| Dibenzyl ether                     | 6.27  | Tribromomethane                                 | 14.4       |
| 1,2-Dibromoethane                  | 12.5  | 1,3,3-Trimethyl-2-oxabicyclo-<br>[2.2.2.]octane | 6.7        |
| Diethyl ether                      | 1.79  | Triphenylmethane                                | 12.45      |
| 1,2-Dimethoxybenzene               | 6.38  | Water                                           | 1.86       |
| <i>N,N</i> -Dimethylacetamide      | 4.46  | <i>p</i> -Xylene                                | 4.3        |
| 2,2-Dimethyl-1-propanol            | 11.0  |                                                 |            |
| Dimethyl sulfoxide                 | 4.07  |                                                 |            |
| 1,4-Dioxane                        | 4.63  |                                                 |            |

11.2 DRYING AND HUMIDIFICATION

TABLE 11.3 Drying Agents

| Drying agent                                    | Most useful for                                                    | Residual water,<br>mg H <sub>2</sub> O per liter<br>of dry air (25°C) | Grams water<br>removed per gram<br>of desiccant        | Regeneration,<br>°C |
|-------------------------------------------------|--------------------------------------------------------------------|-----------------------------------------------------------------------|--------------------------------------------------------|---------------------|
| Al <sub>2</sub> O <sub>3</sub>                  | Hydrocarbons                                                       | 0.002–0.005                                                           | 0.2                                                    | 175 (24 h)          |
| Ba(ClO <sub>4</sub> ) <sub>2</sub> <sup>a</sup> | Inert gas streams                                                  | 0.6–0.8                                                               | 0.17                                                   | 140                 |
| BaO                                             | Basic gases: hydrocarbons, aldehydes, alcohols                     | 0.0007–0.003                                                          | 0.12                                                   | 1000                |
| CaC <sub>2</sub> <sup>b</sup>                   | Ethers                                                             |                                                                       | 0.56                                                   | Impossible          |
| CaCl <sub>2</sub> <sup>c</sup>                  | Inert organics                                                     | 0.1–0.2                                                               | 0.15 (1 H <sub>2</sub> O)<br>0.30 (2 H <sub>2</sub> O) | 250                 |
| CaH <sub>2</sub> <sup>d</sup>                   | Hydrocarbons, ethers, amines, esters, higher alcohols              | 1 × 10 <sup>−5</sup>                                                  | 0.85                                                   | Impossible          |
| CaO                                             | Ethers, esters, alcohols, amines                                   | 0.01–0.003                                                            | 0.31                                                   | Difficult, 1000     |
| CaSO <sub>4</sub>                               | Most organic substances                                            | 0.005–0.07                                                            | 0.07                                                   | 225                 |
| Dow Desiccant 812 <sup>e</sup>                  | Most materials                                                     | (5–200 ppm)                                                           |                                                        | No                  |
| K <sub>2</sub> CO <sub>3</sub>                  | Most materials except acids and phenols                            |                                                                       | 0.16                                                   | 158                 |
| KOH                                             | Amines                                                             | 0.01–0.9                                                              |                                                        | Impossible          |
| LiAlH <sub>4</sub> <sup>f</sup>                 | Hydrocarbons                                                       |                                                                       | 1.9                                                    | Impossible          |
| Mg(ClO <sub>4</sub> ) <sub>2</sub> <sup>a</sup> | Gas streams                                                        | 0.0005–0.002                                                          | 0.24                                                   | 250 (high vacuum)   |
| MgO                                             | All but acidic compounds                                           | 0.008                                                                 | 0.45                                                   | 800                 |
| MgSO <sub>4</sub>                               | Most organic compounds                                             | 1–12                                                                  | 0.15–0.75                                              | Not feasible        |
| Molecular sieves: 4X<br>5X                      | Molecules with effective diameter >4Å                              | 0.001                                                                 | 0.18                                                   | 250                 |
|                                                 | Molecules with effective diameter >5Å                              | 0.001                                                                 | 0.18                                                   | 250                 |
|                                                 | Hydrocarbons, ethers                                               | (For solvents only)                                                   | 0.08                                                   | Impossible          |
| 9.5% Na-Pb alloy <sup>d</sup>                   | Ketones, acids, alkyl and aryl halides                             | 12                                                                    | 1.25                                                   | 150                 |
| Na <sub>2</sub> SO <sub>4</sub>                 | Gas streams; not suitable for alcohols, amines, ketones, or amines | 2 × 10 <sup>−5</sup>                                                  | 0.5                                                    | Not feasible        |
| P <sub>2</sub> O <sub>5</sub>                   |                                                                    |                                                                       |                                                        |                     |
| Silica gel                                      | Most organic amines                                                | 0.002–0.07                                                            | 0.2                                                    | 200–350             |
| Sulfuric acid                                   | Air and inert gas streams                                          | 0.003–0.008                                                           | Indefinite                                             | Not feasible        |

<sup>a</sup> May form explosive mixtures when contacting organic material. <sup>b</sup> Explosive C<sub>2</sub>H<sub>2</sub> formed. <sup>c</sup> Slow in drying action.  
<sup>d</sup> H<sub>2</sub> formed. <sup>e</sup> Used as column drying of organic liquids. <sup>f</sup> Strong reductant.



A saturated aqueous solution in contact with an excess of a definite solid phase at a given temperature will maintain constant humidity in an enclosed space. Table 11.4 gives a number of salts suitable for this purpose. The aqueous tension (vapor pressure, in millimeters of Hg) of a solution at a given temperature is found by multiplying the decimal fraction of the humidity by the aqueous tension at 100 percent humidity for the specific temperature. For example, the aqueous tension of a saturated solution of NaCl at 20°C is  $0.757 \times 17.54 = 13.28$  mmHg and at 80°C it is  $0.764 \times 355.1 = 271.3$  mmHg.

**TABLE 11.4** Solutions for Maintaining Constant Humidity

| Solid Phase                                                         | % Humidity at Specified Temperatures (°C) |       |       |       |       |       |       |
|---------------------------------------------------------------------|-------------------------------------------|-------|-------|-------|-------|-------|-------|
|                                                                     | 10                                        | 20    | 25    | 30    | 40    | 60    | 80    |
| K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>                       |                                           |       | 98.0  |       |       |       |       |
| K <sub>2</sub> SO <sub>4</sub>                                      | 98                                        | 97    | 97    | 96    | 96    | 96    |       |
| KNO <sub>3</sub>                                                    | 95                                        | 93    | 92.5  | 91    | 88    | 82    |       |
| KCl                                                                 | 88                                        | 85.0  | 84.3  | 84    | 81.7  | 80.7  | 79.5  |
| KBr                                                                 |                                           | 84    | 80.7  |       | 79.6  | 79.0  | 79.3  |
| NaCl                                                                | 76                                        | 75.7  | 75.3  | 74.9  | 74.7  | 74.9  | 76.4  |
| NaNO <sub>3</sub>                                                   |                                           |       | 73.8  | 72.8  | 71.5  | 67.5  | 65.5  |
| NaNO <sub>2</sub>                                                   |                                           | 66    | 65    | 63.0  | 61.5  | 59.3  | 58.9  |
| NaBr · 2H <sub>2</sub> O                                            |                                           | 57.9  | 57.7  |       | 52.4  | 49.9  | 50.0  |
| Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> · 2H <sub>2</sub> O  | 58                                        | 55    | 54    |       | 53.6  | 55.2  | 56.0  |
| Mg(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O               | 57                                        | 55    | 52.9  | 52    | 49    | 43    |       |
| K <sub>2</sub> CO <sub>3</sub> · 2H <sub>2</sub> O                  | 47                                        | 44    | 42.8  |       | 42    |       |       |
| MgCl <sub>2</sub> · 6H <sub>2</sub> O                               | 34                                        | 33    | 33.0  | 33    | 32    | 30    |       |
| KF · 2H <sub>2</sub> O                                              |                                           |       |       | 27.4  | 22.8  | 21.0  | 22.8  |
| KC <sub>2</sub> H <sub>3</sub> O <sub>2</sub> · 1.5H <sub>2</sub> O | 24                                        | 23    | 22.5  | 22    | 20    |       |       |
| LiCl · H <sub>2</sub> O                                             | 13                                        | 12    | 10.2  | 12    | 11    | 11    |       |
| KOH                                                                 | 13                                        | 9     | 8     | 7     | 6     | 5     |       |
| 100% Humidity: Aqueous Tension (mm Hg)                              | 9.21                                      | 17.54 | 23.76 | 31.82 | 55.32 | 149.4 | 355.1 |

**TABLE 11.5** Concentrations of Solutions of  $\text{H}_2\text{SO}_4$ ,  $\text{NaOH}$ , and  $\text{CaCl}_2$  Giving Specified Vapor Pressures and Percent Humidities at  $25^\circ\text{C}$ 

| Percent humidity | Aqueous tension, mmHg | $\text{H}_2\text{SO}_4$ |          | $\text{NaOH}$ |          | $\text{CaCl}_2$ |          |
|------------------|-----------------------|-------------------------|----------|---------------|----------|-----------------|----------|
|                  |                       | Molality                | Weight % | Molality      | Weight % | Molality        | Weight % |
| 100              | 23.76                 | 0.00                    | 0.00     | 0.00          | 0.00     | 0.00            | 0.00     |
| 95               | 22.57                 | 1.263                   | 11.02    | 1.465         | 5.54     | 0.927           | 9.33     |
| 90               | 21.38                 | 2.224                   | 17.91    | 2.726         | 9.83     | 1.584           | 14.95    |
| 85               | 20.19                 | 3.025                   | 22.88    | 3.840         | 13.32    | 2.118           | 19.03    |
| 80               | 19.00                 | 3.730                   | 26.79    | 4.798         | 16.10    | 2.579           | 22.25    |
| 75               | 17.82                 | 4.398                   | 30.14    | 5.710         | 18.60    | 2.995           | 24.95    |
| 70               | 16.63                 | 5.042                   | 33.09    | 6.565         | 20.80    | 3.400           | 27.40    |
| 65               | 15.44                 | 5.686                   | 35.80    | 7.384         | 22.80    | 3.796           | 29.64    |
| 60               | 14.25                 | 6.341                   | 38.35    | 8.183         | 24.66    | 4.188           | 31.73    |
| 55               | 13.07                 | 7.013                   | 40.75    | 8.974         | 26.42    | 4.581           | 33.71    |
| 50               | 11.88                 | 7.722                   | 43.10    | 9.792         | 28.15    | 4.990           | 35.64    |
| 45               | 10.69                 | 8.482                   | 45.41    | 10.64         | 29.86    | 5.431           | 37.61    |
| 40               | 9.50                  | 9.304                   | 47.71    | 11.54         | 31.58    | 5.912           | 39.62    |
| 35               | 8.31                  | 10.21                   | 50.04    | 12.53         | 33.38    | 6.478           | 41.83    |
| 30               | 7.13                  | 11.25                   | 52.45    | 13.63         | 35.29    | 7.183           | 44.36    |
| 25               | 5.94                  | 12.47                   | 55.01    | 14.96         | 37.45    |                 |          |
| 20               | 4.75                  | 13.94                   | 57.76    | 16.67         | 40.00    |                 |          |
| 15               | 3.56                  | 15.81                   | 60.80    | 19.10         | 43.32    |                 |          |
| 10               | 2.38                  | 18.48                   | 64.45    | 23.05         | 47.97    |                 |          |
| 5                | 1.19                  | 23.17                   | 69.44    |               |          |                 |          |

Concentrations are expressed in percentage of anhydrous solute by weight.

**Source:** Stokes and Robinson, *Ind. Eng. Chem.* **41**:2013 (1949).

TABLE 11.6 Relative Humidity from Wet and Dry Bulb Thermometer Readings

| Dry bulb temperature, °C | Wet bulb depression, °C |     |     |     |     |     |      |      |      |      |      |      |
|--------------------------|-------------------------|-----|-----|-----|-----|-----|------|------|------|------|------|------|
|                          | 0.5                     | 1.0 | 1.5 | 2.0 | 2.5 | 3.0 | 3.5  | 4.0  | 4.5  | 5.0  | 5.5  | 6.0  |
|                          | Relative humidity, %    |     |     |     |     |     |      |      |      |      |      |      |
| −10                      | 83                      | 67  | 51  | 35  | 19  |     |      |      |      |      |      |      |
| −5                       | 88                      | 76  | 64  | 52  | 41  | 29  | 18   | 7    |      |      |      |      |
| 0                        | 91                      | 81  | 72  | 64  | 55  | 46  | 38   | 29   | 21   | 13   | 5    |      |
| 2                        | 91                      | 84  | 76  | 68  | 60  | 52  | 44   | 37   | 29   | 22   | 14   | 7    |
| 4                        | 92                      | 85  | 78  | 71  | 63  | 57  | 49   | 43   | 36   | 29   | 22   | 16   |
| 6                        | 93                      | 86  | 79  | 73  | 66  | 60  | 54   | 48   | 41   | 35   | 29   | 24   |
| 8                        | 93                      | 87  | 81  | 75  | 69  | 63  | 57   | 51   | 46   | 40   | 35   | 29   |
| 10                       | 94                      | 88  | 82  | 77  | 71  | 66  | 60   | 55   | 50   | 44   | 39   | 34   |
| 12                       | 94                      | 89  | 83  | 78  | 73  | 68  | 63   | 58   | 53   | 48   | 43   | 39   |
| 14                       | 95                      | 90  | 85  | 79  | 75  | 70  | 65   | 60   | 56   | 51   | 47   | 42   |
| 16                       | 95                      | 90  | 85  | 81  | 76  | 71  | 67   | 63   | 58   | 54   | 50   | 46   |
| 18                       | 95                      | 91  | 86  | 82  | 77  | 73  | 69   | 65   | 61   | 57   | 53   | 49   |
| 20                       | 96                      | 91  | 87  | 83  | 78  | 74  | 70   | 66   | 63   | 59   | 55   | 51   |
| 22                       | 96                      | 92  | 87  | 83  | 80  | 76  | 72   | 68   | 64   | 61   | 57   | 54   |
| 24                       | 96                      | 92  | 88  | 84  | 80  | 77  | 73   | 69   | 66   | 62   | 59   | 56   |
| 26                       | 96                      | 92  | 88  | 85  | 81  | 78  | 74   | 71   | 67   | 64   | 61   | 58   |
| 28                       | 96                      | 93  | 89  | 85  | 82  | 78  | 75   | 72   | 69   | 65   | 62   | 59   |
| 30                       | 96                      | 93  | 89  | 86  | 83  | 79  | 76   | 73   | 70   | 67   | 64   | 61   |
| 35                       | 97                      | 94  | 90  | 87  | 84  | 81  | 78   | 75   | 72   | 69   | 67   | 64   |
| 40                       | 97                      | 94  | 91  | 88  | 85  | 82  | 80   | 77   | 74   | 72   | 69   | 67   |
| Dry bulb temperature, °C | Wet bulb depression, °C |     |     |     |     |     |      |      |      |      |      |      |
|                          | 6.5                     | 7.0 | 7.5 | 8.0 | 8.5 | 9.0 | 10.0 | 11.0 | 12.0 | 13.0 | 14.0 | 15.0 |
|                          | Relative humidity, %    |     |     |     |     |     |      |      |      |      |      |      |
| 4                        | 9                       |     |     |     |     |     |      |      |      |      |      |      |
| 6                        | 17                      | 11  | 5   |     |     |     |      |      |      |      |      |      |
| 8                        | 24                      | 19  | 14  | 8   |     |     |      |      |      |      |      |      |
| 10                       | 29                      | 24  | 20  | 15  | 10  | 6   |      |      |      |      |      |      |
| 12                       | 34                      | 29  | 25  | 21  | 16  | 12  | 5    |      |      |      |      |      |
| 14                       | 38                      | 34  | 30  | 26  | 22  | 18  | 10   |      |      |      |      |      |
| 16                       | 42                      | 38  | 34  | 30  | 26  | 23  | 15   | 8    |      |      |      |      |
| 18                       | 45                      | 41  | 38  | 34  | 30  | 27  | 20   | 14   | 7    |      |      |      |
| 20                       | 48                      | 44  | 41  | 37  | 34  | 31  | 24   | 18   | 12   | 6    |      |      |
| 22                       | 50                      | 47  | 44  | 40  | 37  | 34  | 28   | 22   | 17   | 11   | 6    |      |
| 24                       | 53                      | 49  | 46  | 43  | 40  | 37  | 31   | 26   | 20   | 15   | 10   | 5    |
| 26                       | 54                      | 51  | 49  | 46  | 43  | 40  | 34   | 29   | 24   | 19   | 14   | 10   |
| 28                       | 56                      | 53  | 51  | 48  | 45  | 42  | 37   | 32   | 27   | 22   | 18   | 13   |
| 30                       | 58                      | 55  | 52  | 50  | 47  | 44  | 39   | 35   | 30   | 25   | 21   | 17   |
| 32                       | 60                      | 57  | 54  | 51  | 49  | 46  | 41   | 37   | 32   | 28   | 24   | 20   |
| 34                       | 61                      | 58  | 56  | 53  | 51  | 48  | 43   | 39   | 35   | 30   | 26   | 23   |
| 36                       | 62                      | 59  | 57  | 54  | 52  | 50  | 45   | 41   | 37   | 33   | 29   | 25   |
| 38                       | 63                      | 61  | 58  | 56  | 54  | 51  | 47   | 43   | 39   | 35   | 31   | 27   |
| 40                       | 64                      | 62  | 59  | 57  | 54  | 53  | 48   | 44   | 40   | 36   | 33   | 29   |

**TABLE 11.7** Relative Humidity from Dew Point Readings

| Depression of<br>dew point,<br>°C | Dew point reading, °C |    |    |    |    |
|-----------------------------------|-----------------------|----|----|----|----|
|                                   | − 10                  | 0  | 10 | 20 | 30 |
|                                   | Relative humidity, %  |    |    |    |    |
| 0.5                               | 96                    | 96 | 96 | 96 | 97 |
| 1.0                               | 92                    | 93 | 94 | 94 | 94 |
| 1.5                               | 89                    | 89 | 90 | 91 | 92 |
| 2.0                               | 86                    | 87 | 88 | 88 | 89 |
| 3.0                               | 79                    | 81 | 82 | 83 | 84 |
| 4.0                               | 73                    | 75 | 77 | 78 | 80 |
| 5.0                               | 68                    | 70 | 72 | 74 | 75 |
| 6.0                               | 63                    | 66 | 68 | 70 | 71 |
| 7.0                               | 59                    | 61 | 63 | 66 | 68 |
| 8.0                               | 54                    | 57 | 60 | 62 | 64 |
| 9.0                               | 51                    | 53 | 56 | 58 | 61 |
| 10.0                              | 47                    | 50 | 53 | 55 | 57 |
| 11.0                              | 44                    | 47 | 49 | 52 |    |
| 12.0                              | 41                    | 44 | 47 | 49 |    |
| 13.0                              | 38                    | 41 | 44 | 46 |    |
| 14.0                              | 35                    | 38 | 41 | 44 |    |
| 15.0                              | 33                    | 36 | 39 | 42 |    |
| 16.0                              | 31                    | 34 | 37 | 39 |    |
| 18.0                              | 27                    | 30 | 33 | 35 |    |
| 20.0                              | 24                    | 26 | 29 | 32 |    |
| 22.0                              | 21                    | 23 | 26 |    |    |
| 24.0                              | 18                    | 21 | 23 |    |    |
| 26.0                              | 16                    | 18 | 21 |    |    |
| 28.0                              | 14                    | 16 | 19 |    |    |
| 30.0                              | 12                    | 14 | 17 |    |    |

### 11.3 BOILING POINTS AND HEATING BATHS

**TABLE 11.8** Organic Solvents Arranged by Boiling Points

| Name                     | BP, °C | Name                      | BP, °C |
|--------------------------|--------|---------------------------|--------|
| Ethylene oxide           | 10.6   | 1-Propanol                | 97.2   |
| Chloroethane             | 12.3   | Heptane                   | 98.4   |
| Furan                    | 31.4   | 1-Chloro-3-methylbutane   | 99     |
| Methyl formate           | 31.5   | Ethyl propionate          | 99.1   |
| Diethyl ether            | 34.6   | 2-Butanol                 | 99.6   |
| Propylene oxide          | 34.5   | Formic acid               | 100.8  |
| Pentane                  | 36.1   | Methylcyclohexane         | 100.9  |
| Bromoethane              | 38.4   | 1,4-Dioxane               | 101.2  |
| Dichloromethane          | 39.8   | Nitromethane              | 101.2  |
| Dimethoxymethane         | 42.3   | Propyl acetate            | 101.5  |
| Carbon disulfide         | 46.3   | 2-Pentanone               | 101.7  |
| 1-Isopropoxy-2-propanol  | 47.9   | 3-Pentanone               | 102.0  |
| Ethyl formate            | 54.2   | 2-Methyl-2-butanol        | 102.0  |
| Acetone                  | 56.2   | 1,1-Diethoxyethane        | 102.7  |
| Methyl acetate           | 56.3   | Butyl formate             | 106.6  |
| 1,1-Dichloroethane       | 57.3   | 2-Methyl-1-propanol       | 107.9  |
| Dichloroethylene         | 60.6   | Toluene                   | 110.6  |
| Chloroform               | 61.2   | sec-Butyl acetate         | 112.3  |
| Methanol                 | 64.7   | 1,1,2-Trichloroethane     | 113.5  |
| Tetrahydrofuran          | 66.0   | Nitroethane               | 114.1  |
| Diisopropyl ether        | 68.0   | Pyridine                  | 115.2  |
| Hexane                   | 68.7   | 3-Pentanol                | 115.6  |
| 1-Chloro-2-methylpropane | 68.9   | 4-Methyl-2-pentanone      | 115.7  |
| 1,1,1-Trichloroethane    | 74.0   | 1-Chloro-2,3-epoxypropane | 116.1  |
| 1,3-Dioxolane            | 74–75  | 1-Butanol                 | 117.7  |
| Carbon tetrachloride     | 76.7   | Acetic acid               | 117.9  |
| Ethyl acetate            | 77.1   | Isobutyl acetate          | 118.0  |
| 1-Chlorobutane           | 77.9   | 2-Pentanol                | 119.3  |
| Ethanol                  | 78.3   | 1-Bromo-3-methylbutane    | 119.7  |
| 2-Butanone               | 79.6   | 1-Methoxy-2-propanol      | 120.1  |
| 2-Methyltetrahydrofuran  | 80.0   | 2-Nitropropane            | 120.3  |
| Benzene                  | 80.1   | Tetrachloroethylene       | 121.1  |
| Cyclohexane              | 80.7   | Ethyl butyrate            | 121.6  |
| Propyl formate           | 80.9   | 3-Hexanone                | 123    |
| Acetonitrile             | 81.6   | 2,4-Dimethyl-3-pentanone  | 124    |
| 2-Propanol               | 82.4   | 2-Methoxyethanol          | 124.6  |
| 1,1,-Dimethylethanol     | 82.4   | Octane                    | 125.7  |
| Cyclohexene              | 83.0   | Butyl acetate             | 126.1  |
| Diisopropylamine         | 83.5   | Diethyl carbonate         | 126.8  |
| 1,2-Dichloroethane       | 83.7   | 2-Hexanone                | 127.2  |
| Thiophene                | 84.2   | 1-Chloro-2-propanol       | 127.4  |
| Trichloroethylene        | 87.2   | 2-Chloroethanol           | 128.6  |
| Isopropyl acetate        | 88.2   | 3-Methyl-1-penten-2-one   | 129.5  |
| 1-Bromo-2-methylpropane  | 91.5   | 1-Nitropropane            | 131.2  |
| 2,5-Dimethylfuran        | 93–94  | Chlorobenzene             | 131.7  |
| Ethyl chloroformate      | 94     | 1,2-Dibromoethane         | 131.7  |
| Allyl alcohol            | 96.6   | 4-Methyl-2-pentanol       | 131.7  |
| 1,2-Dichloropropane      | 96.8   |                           |        |

**TABLE 11.8** Organic Solvents Arranged by Boiling Points (*Continued*)

| Name                                       | BP, °C  | Name                               | BP, °C  |
|--------------------------------------------|---------|------------------------------------|---------|
| 3-Methyl-1-butanol                         | 132.0   | 2-Octanol                          | 179     |
| Cyclohexylamine                            | 134.8   | 1,2-Dichlorobenzene                | 180.4   |
| 2-Ethoxyethanol                            | 134.8   | Ethyl acetoacetate                 | 180.8   |
| Ethylbenzene                               | 136.2   | Phenol                             | 181.8   |
| 1-Pentanol                                 | 138     | 2-Ethyl-1-hexanol                  | 184.3   |
| <i>p</i> -Xylene                           | 138.4   | Aniline                            | 184.4   |
| <i>m</i> -Xylene                           | 139.1   | Benzyl ethyl ether                 | 185.0   |
| Acetic anhydride                           | 140.0   | Diethyl oxalate                    | 185.4   |
| 2,4-Pentanedione                           | 140.6   | 1,2-Propanediol                    | 188     |
| Isopentyl acetate                          | 142     | Bis(2-ethoxyethyl) ether           | 188.4   |
| Dibutyl ether                              | 142.4   | Dimethyl sulfoxide                 | 189.0   |
| 4-Heptanone                                | 143.7   | 1,2-Ethanediol diacetate           | 190.2   |
| <i>o</i> -Xylene                           | 144.4   | Benzonitrile                       | 191.0   |
| 2-Methoxyethyl acetate                     | 144.5   | 2,5-Hexanedione                    | 191.4   |
| 1,1,2,2-Tetrachloroethane                  | 146.3   | 2-(2-Methoxyethoxy)-ethanol        | 194.1   |
| 3-Heptanone                                | 147.8   | <i>N,N</i> -Dimethylaniline        | 194.2   |
| Tribromomethane                            | 149.6   | 1-Octanol                          | 195.2   |
| Nonane                                     | 150.8   | 1,2-Ethanediol                     | 197.3   |
| 2-Heptanone                                | 151     | Diethyl malonate                   | 199.3   |
| Isopropylbenzene                           | 152.4   | Methyl benzoate                    | 199.5   |
| <i>N,N</i> -Dimethylformamide              | 153.0   | <i>o</i> -Toluidine                | 200.4   |
| Methoxybenzene                             | 153.8   | <i>p</i> -Toluidine                | 200.6   |
| Ethyl lactate                              | 154.5   | 2-(2-Ethoxyethoxy)-ethanol         | 202     |
| Cyclohexanone                              | 155.7   | Acetophenone                       | 202.1   |
| Bromobenzene                               | 156.2   | 1,2-Dibutoxyethane                 | 203.6   |
| 1,2,3-Trichloropropane                     | 156.9   | 1-Phenylethanol                    | 203.9   |
| 1-Hexanol                                  | 157.5   | <i>m</i> -Toluidine                | 203.4   |
| Propylbenzene                              | 159.2   | Benzyl alcohol                     | 205.5   |
| Cyclohexanol                               | 161.1   | Camphor                            | 207     |
| Bis(2-methoxyethyl)ether                   | 160     | 1,3-Butanediol                     | 207.5   |
| Isopentyl propionate                       | 160.2   | 1,2,3,4-Tetrahydro-naphthalene     | 207.6   |
| 2-Heptanol                                 | 160.4   | $\gamma$ -Valerolactone            | 207–208 |
| Pentachloroethane                          | 160.5   | <i>o</i> -Chloroaniline            | 208.8   |
| 2-Furaldehyde                              | 161.8   | Nitrobenzene                       | 210.8   |
| 2,6-Dimethyl-4-heptanone                   | 168.1   | Ethyl benzoate                     | 212.4   |
| 4-Hydroxy-4-methyl-2-pentanone             | 169.2   | 3,5,5-Trimethylcyclohex-2-en-1-one | 215.2   |
| 2-Furanmethanol                            | 170.0   | Naphthalene                        | 217.7   |
| Ethoxybenzene                              | 170     | 2-(2-Ethoxyethoxy)ethyl acetate    | 218.5   |
| 2-Butoxyethanol                            | 170.2   | Acetamide                          | 221.2   |
| Diisopentyl ether                          | 173.4   | Methyl salicylate                  | 223.0   |
| Decane                                     | 174.2   | Diethyl maleate                    | 225.3   |
| 1,3-Dichloro-2-propanol                    | 174.3   | 1,4-Butanediol                     | 230     |
| Cyclohexyl acetate                         | 174–175 | Propyl benzoate                    | 231.2   |
| 1-Heptanol                                 | 175.8   | 1-Decanol                          | 230.2   |
| Furfuryl acetate                           | 175–177 | Phenylacetone nitrile              | 233.5   |
| 1,3,3-Trimethyl-2-oxabicyclo-[2.2.2]octane | 177.4   | Quinoline                          | 237     |
| 4-Isopropyl-1-methylbenzene                | 177.1   | Tributyl borate                    | 238.5   |
| Isopentyl butyrate                         | 178.6   | Propylene carbonate                | 240     |
| Bis(2-chloroethyl) ether                   | 178.8   |                                    |         |

**TABLE 11.8** Organic Solvents Arranged by Boiling Points (*Continued*)

| Name                              | BP, °C  | Name                            | BP, °C  |
|-----------------------------------|---------|---------------------------------|---------|
| 2-Phenoxyethanol                  | 240     | Isopentyl salicylate            | 277–278 |
| Bis(2-hydroxyethyl) ether         | 245     | 1-Bromonaphthalene              | 281.1   |
| Dibutyl oxalate                   | 245.5   | Dimethyl <i>o</i> -phthalate    | 283.7   |
| Butyl benzoate                    | 250     | 2,2'-(Ethylenedioxy)-bisethanol | 285     |
| 1,2,3-Propanetriol triacetate     | 258–259 | Glycerol                        | 290     |
| 1-Chloronaphthalene               | 259.3   | Diethyl <i>o</i> -phthalate     | 295     |
| Isopentyl benzoate                | 262     | Benzyl benzoate                 | 323.5   |
| <i>trans</i> -Ethyl cinnamate     | 271.0   | Dibutyl <i>o</i> -phthalate     | 340.0   |
| Bis[2-(methoxyethoxy)-ethyl]ether | 275.3   | Dibutyl decanedioate            | 344–345 |
| 1-Methoxy-2-nitrobenzene          | 277     |                                 |         |

**TABLE 11.9** Molecular Elevation of the Boiling Point*Ebullioscopic constants.*

Molecular weights can be determined with the relation:

$$M = E_b \frac{1000 w_2}{w_1 \Delta T_b}$$

where  $\Delta T_b$  is the elevation of the boiling point brought about by the addition of  $w_2$  grams of solute to  $w_1$  grams of solvent and  $E_b$  is the ebullioscopic constant. In the column headed "Barometric correction" is the number of degrees for each millimeter of difference between the barometric reading and 760 mmHg to be subtracted from  $E_b$  if the pressure is lower, or added if higher, than 760 mm. In general, the effect is within experimental error if the pressure is within 10 mm of 760 mm.

The ebullioscopic constant, a characteristic property of the solvent, may be calculated from the relation:

$$E_b = \frac{RT_b^2 M}{\Delta_{vap} H}$$

where  $R$  is the molar gas constant,  $M$  is the molar mass of the solvent, and  $\Delta_{vap} H$  the molar enthalpy (heat) of vaporization of the solvent.

| Compound              | Barometric correction | $E_b$ ,<br>°C kg · mol <sup>-1</sup> |
|-----------------------|-----------------------|--------------------------------------|
| Acetic acid           | 0.0008                | 3.22                                 |
| Acetic anhydride      |                       | 3.79                                 |
| Acetone               | 0.0004                | 1.80                                 |
| Acetonitrile          |                       | 1.44                                 |
| Acetophenone          |                       | 5.81                                 |
| Aniline               | 0.0009                | 3.82                                 |
| Benzaldehyde          |                       | 4.24                                 |
| Benzene               | 0.0007                | 2.64                                 |
| Benzonitrile          |                       | 4.02                                 |
| Bromobenzene          | 0.0016                | 6.35                                 |
| Bromoethane           |                       | 1.73                                 |
| 1-Butanol             |                       | 2.17                                 |
| 2-Butanone            |                       | 2.28                                 |
| cis-2-Butene-1,4-diol |                       | 2.73                                 |
| D-(+)-Camphor         | 0.0015                | 4.91                                 |
| Carbon disulfide      | 0.0006                | 2.42                                 |
| Carbon tetrachloride  | 0.0013                | 5.26                                 |
| Chlorobenzene         | 0.0011                | 4.36                                 |
| 1-Chlorobutane        |                       | 3.13                                 |
| Chloroethane          |                       | 1.77                                 |
| Chloroform            | 0.0009                | 3.80                                 |
| Cyclohexane           | 0.0007                | 2.92                                 |
| Cyclohexanol          |                       | 3.5                                  |
| Decane                |                       | 6.10                                 |
| 1,2-Dibromomethane    | 0.0016                | 6.01                                 |
| 1,1-Dichloroethane    |                       | 3.13                                 |
| 1,2-Dichloroethane    |                       | 3.27                                 |
| Dichloromethane       |                       | 2.42                                 |
| Diethyl ether         | 0.0005                | 2.20                                 |
| Diethyl sulfide       |                       | 3.14                                 |
| Dimethoxymethane      |                       | 2.12                                 |
| N,N-Dimethylacetamide |                       | 3.22                                 |
| Dimethyl sulfide      |                       | 1.85                                 |
| Dimethyl sulfoxide    |                       | 3.22                                 |



**TABLE 11.9** Molecular Elevation of the Boiling Point (*Continued*)

| Compound                              | Barometric<br>correction | $E_b$ ,<br>°C kg · mol <sup>-1</sup> |
|---------------------------------------|--------------------------|--------------------------------------|
| 1,4-Dioxane                           |                          | 3.00                                 |
| Ethanol                               | 0.0003                   | 1.22                                 |
| Ethoxybenzene                         |                          | 4.90                                 |
| Ethyl acetate                         | 0.0007                   | 2.82                                 |
| Ethylene glycol                       |                          | 2.26                                 |
| Formic acid                           |                          | 2.36                                 |
| Glycerol                              |                          | 6.52                                 |
| Heptane                               | 0.0008                   | 3.62                                 |
| Hexane                                |                          | 2.90                                 |
| 2-Hydroxybenzaldehyde                 |                          | 5.87                                 |
| Iodoethane                            |                          | 5.27                                 |
| Iodomethane                           |                          | 4.31                                 |
| 4-Isopropyl-1-methylbenzene           |                          | 5.92                                 |
| Methanol                              | 0.0002                   | 0.86                                 |
| Methoxybenzene                        |                          | 4.20                                 |
| Methyl acetate                        | 0.0005                   | 2.21                                 |
| <i>N</i> -Methylaniline               |                          | 4.3                                  |
| 2-Methyl-2-butanol                    |                          | 2.64                                 |
| 3-Methyl-1-butanol                    |                          | 2.88                                 |
| 3-Methylbutyl acetate                 |                          | 4.83                                 |
| <i>N</i> -Methylformamide             |                          | 2.2                                  |
| Methyl formate                        |                          | 1.66                                 |
| 2-Methyl-1-propanol                   |                          | 2.14                                 |
| 2-Methyl-2-propanol                   |                          | 1.99                                 |
| Naphthalene                           | 0.0014                   | 5.94                                 |
| Nitrobenzene                          |                          | 5.24                                 |
| Nitroethane                           |                          | 2.46                                 |
| Nitromethane                          |                          | 2.09                                 |
| Octane                                |                          | 4.39                                 |
| 1-Octanol                             |                          | 5.06                                 |
| Pentyl acetate                        |                          | 4.71                                 |
| Phenol                                | 0.0009                   | 3.54                                 |
| Piperidine                            |                          | 3.21                                 |
| Propanoic acid                        |                          | 3.27                                 |
| 1-Propanol                            |                          | 1.66                                 |
| 2-Propanol                            |                          | 1.58                                 |
| Propionitrile                         |                          | 1.97                                 |
| Pyridine                              |                          | 2.83                                 |
| Pyrrole                               |                          | 2.33                                 |
| Pyrrolidine                           |                          | 2.32                                 |
| Quinoline                             |                          | 5.62                                 |
| Tetrachloroethylene                   |                          | 6.18                                 |
| Tetrachloromethane                    |                          | 5.26                                 |
| 1,2,3,4-Tetrahydronaphthalene         |                          | 5.58                                 |
| Toluene                               | 0.0008                   | 3.40                                 |
| <i>p</i> -Toluidine                   |                          | 4.51                                 |
| Trichloroethylene                     |                          | 4.52                                 |
| Trichloromethane                      | 0.0009                   | 3.80                                 |
| 1,1,2-Trichloro-1,2,2-trifluoroethane |                          | 5.93                                 |
| Triethylamine                         |                          | 3.57                                 |
| Water                                 | 0.0001                   | 0.512                                |
| <i>o</i> -Xylene                      |                          | 4.25                                 |

**TABLE 11.10** Substances Which Can Be Used for Heating Baths

| Medium                      | Melting point, °C | Boiling point, °C | Useful range, °C | Flash point, °C | Comments                            |
|-----------------------------|-------------------|-------------------|------------------|-----------------|-------------------------------------|
| Water                       | 0                 | 100               | 0–100            | None            | Ideal                               |
| Silicone oil                | – 50              | —                 | 30–250           | 315             | Somewhat viscous at low temperature |
| Triethylene glycol          | – 7               | 285               | 0–250            | 165             | Noncorrosive                        |
| Glycerol                    | 18                | 290               | – 20 to 260      | 160             | Water-soluble, nontoxic             |
| Paraffin                    | 50                | —                 | 60–300           | 199             | Flammable                           |
| Dibutyl <i>o</i> -phthalate | – 35              | 340               | 150–320          | 171             | Generally used                      |

TABLE 11.11 Solvents of Chromatographic Interest

| Solvent                | Boiling point, °C | Solvent strength parameter |                                      | Viscosity, mN · s · m <sup>-2</sup> (20°C) | Refractive index (20°C) | UV cutoff, nm |
|------------------------|-------------------|----------------------------|--------------------------------------|--------------------------------------------|-------------------------|---------------|
|                        |                   | e° (SiO <sub>2</sub> )     | e° (Al <sub>2</sub> O <sub>3</sub> ) |                                            |                         |               |
| Fluoroalkanes          |                   |                            | − 0.25                               |                                            | 1.25                    |               |
| Pentane                | 36                | 0.0                        | 0.0                                  | 0.24 <sup>15°C</sup>                       | 1.358                   | 210           |
| Hexane                 | 69                | 0.0                        | 0.0                                  | 0.31                                       | 1.375                   | 210           |
| 2,2,4-Trimethylpentane | 99                |                            | 0.01                                 | 0.50                                       | 1.392                   | 215           |
| Decane                 | 174               |                            | 0.04                                 | 0.93                                       | 1.412                   | 210           |
| Cyclohexane            | 81                | − 0.05                     | 0.04                                 | 0.98                                       | 1.426                   | 210           |
| Cyclopentane           | 49                |                            | 0.05                                 | 0.44                                       | 1.407                   | 210           |
| Diisobutylene          | 101               |                            | 0.06                                 |                                            | 1.411                   |               |
| 1-Pentene              | 30                |                            | 0.08                                 | 0.24 <sup>0°C</sup>                        | 1.371                   |               |
| Carbon disulfide       | 46                | 0.14                       | 0.15                                 | 0.36                                       | 1.626                   | 380           |
| Carbon tetrachloride   | 77                | 0.14                       | 0.18                                 | 0.97                                       | 1.466                   | 265           |
| 1-Chlorobutane         | 78                |                            | 0.26                                 | 0.43                                       | 1.402                   | 220           |
| 1-Chloropentane        | 98                |                            | 0.26                                 | 0.58                                       | 1.412                   | 225           |
| o-Xylene               | 144               |                            | 0.26                                 | 0.81                                       | 1.505                   | 290           |
| Diisopropyl ether      | 68                |                            | 0.28                                 | 0.38 <sup>25°C</sup>                       | 1.369                   | 220           |
| 2-Chloropropane        | 35                |                            | 0.29                                 | 0.33                                       | 1.378                   | 225           |
| Toluene                | 111               |                            | 0.29                                 | 0.59                                       | 1.497                   | 286           |
| 1-Chloropropane        | 47                |                            | 0.30                                 | 0.35                                       | 1.389                   | 225           |
| Chlorobenzene          | 132               |                            | 0.40                                 | 0.80                                       | 1.525                   |               |
| Benzene                | 80                | 0.25                       | 0.32                                 | 0.65                                       | 1.501                   | 280           |
| Bromoethane            | 38                |                            | 0.37                                 | 0.40                                       | 1.424                   |               |

**TABLE 11.11** Solvents of Chromatographic Interest     *Continued*

| Solvent              | Boiling point, °C | Solvent strength parameter                |                                                         | Viscosity, mN · s · m <sup>-2</sup> (20°C) | Refractive index (20°C) | UV cutoff, nm |
|----------------------|-------------------|-------------------------------------------|---------------------------------------------------------|--------------------------------------------|-------------------------|---------------|
|                      |                   | <i>e</i> <sup>o</sup> (SiO <sub>2</sub> ) | <i>e</i> <sup>o</sup> (Al <sub>2</sub> O <sub>3</sub> ) |                                            |                         |               |
| Diethyl ether        | 35                | 0.38                                      | 0.38                                                    | 0.25                                       | 1.353                   | 218           |
| Diethyl sulfide      | 92                |                                           | 0.38                                                    | 0.45                                       | 1.443                   | 290           |
| Chloroform           | 62                | 0.26                                      | 0.40                                                    | 0.57                                       | 1.443                   | 245           |
| Dichloromethane      | 41                |                                           | 0.42                                                    | 0.44                                       | 1.425                   | 235           |
| 4-Methyl-2-pentanone | 116               |                                           | 0.43                                                    | 0.42 <sup>15°C</sup>                       | 1.396                   | 335           |
| Tetrahydrofuran      | 66                |                                           | 0.45                                                    | 0.55                                       | 1.407                   | 220           |
| 1,2-Dichloroethane   | 84                |                                           | 0.49                                                    | 0.80                                       | 1.445                   | 228           |
| 2-Butanone           | 80                |                                           | 0.51                                                    | 0.42 <sup>15°C</sup>                       | 1.379                   | 330           |
| 1-Nitropropane       | 131               |                                           | 0.53                                                    | 0.80 <sup>25°C</sup>                       | 1.402                   | 380           |
| Acetone              | 56                | 0.47                                      | 0.56                                                    | 0.32                                       | 1.359                   | 330           |
| 1,4-Dioxane          | 101               | 0.49                                      | 0.56                                                    | 1.44 <sup>15°C</sup>                       | 1.420                   | 215           |
| Ethyl acetate        | 77                | 0.38                                      | 0.58                                                    | 0.45                                       | 1.372                   | 255           |
| Methyl acetate       | 56                |                                           | 0.60                                                    | 0.48 <sup>15°C</sup>                       | 1.362                   | 260           |
| 1-Pentanol           | 138               |                                           | 0.61                                                    | 4.1                                        | 1.410                   | 210           |
| Dimethyl sulfoxide   | 189               |                                           | 0.62                                                    | 2.47                                       | 1.478                   | 265           |
| Aniline              | 184               |                                           | 0.62                                                    | 4.40                                       | 1.586                   |               |
| Diethylamine         | 56                |                                           | 0.63                                                    | 0.33                                       | 1.386                   | 275           |
| Nitromethane         | 101               |                                           | 0.64                                                    | 0.67                                       | 1.394                   | 380           |
| Acetonitrile         | 82                | 0.50                                      | 0.65                                                    | 0.37                                       | 1.344                   | 190           |
| Pyridine             | 115               |                                           | 0.71                                                    | 0.97                                       | 1.510                   | 330           |
| 2-Butoxyethanol      | 170               |                                           | 0.74                                                    | 3.15 <sup>25°C</sup>                       | 1.420                   | 220           |
| 1-Propanol           | 97                |                                           | 0.82                                                    | 2.25                                       | 1.386                   | 210           |
| 2-Propanol           | 82                |                                           | 0.82                                                    | 2.50                                       | 1.377                   | 210           |
| Ethanol              | 78                |                                           | 0.88                                                    | 1.20                                       | 1.361                   | 210           |
| Methanol             | 65                |                                           | 0.95                                                    | 0.59                                       | 1.328                   | 210           |
| Ethylene glycol      | 198               |                                           | 1.11                                                    | 21.8                                       | 1.432                   | 210           |
| Acetic acid          | 118               |                                           | large                                                   | 1.23                                       | 1.372                   | 260           |
| Water                | 100               |                                           | large                                                   | 1.00                                       | 1.333                   | 191           |

TABLE 11.12 Solvents Having the Same Refractive Index and the Same Density at 25°C

| Solvent 1                | Solvent 2                | Refractive index |       | Density, g/mL |       |
|--------------------------|--------------------------|------------------|-------|---------------|-------|
|                          |                          | 1                | 2     | 1             | 2     |
| Acetone                  | Ethanol                  | 1.357            | 1.359 | 0.788         | 0.786 |
| Ethyl formate            | Methyl acetate           | 1.358            | 1.360 | 0.916         | 0.935 |
| Ethanol                  | Propionitrile            | 1.359            | 1.363 | 0.786         | 0.777 |
| 2,2-Dimethylbutane       | 2-Methylpentane          | 1.366            | 1.369 | 0.644         | 0.649 |
| 2-Methylpentane          | Hexane                   | 1.369            | 1.372 | 0.649         | 0.655 |
| Isopropyl acetate        | 2-Chloropropane          | 1.375            | 1.376 | 0.868         | 0.865 |
| 3-Butanone               | Butyraldehyde            | 1.377            | 1.378 | 0.801         | 0.799 |
| Butyraldehyde            | Butyronitrile            | 1.378            | 1.382 | 0.799         | 0.786 |
| Dipropyl ether           | Butyl ethyl ether        | 1.379            | 1.380 | 0.753         | 0.746 |
| Propyl acetate           | Ethyl propionate         | 1.382            | 1.382 | 0.883         | 0.888 |
| Propyl acetate           | 1-Chloropropane          | 1.382            | 1.386 | 0.883         | 0.890 |
| Butyronitrile            | 2-Methyl-2-propanol      | 1.382            | 1.385 | 0.786         | 0.781 |
| Ethyl propionate         | 1-Chloropropane          | 1.382            | 1.386 | 0.888         | 0.890 |
| 1-Propanol               | 2-Pentanone              | 1.383            | 1.387 | 0.806         | 0.804 |
| Isobutyl formate         | 1-Chloropropane          | 1.383            | 1.386 | 0.881         | 0.890 |
| 1-Chloropropane          | Butyl formate            | 1.386            | 1.387 | 0.890         | 0.888 |
| Butyl formate            | Methyl butyrate          | 1.387            | 1.391 | 0.888         | 0.875 |
| Methyl butyrate          | 2-Chlorobutane           | 1.392            | 1.395 | 0.875         | 0.868 |
| Butyl acetate            | 2-Chlorobutane           | 1.392            | 1.395 | 0.877         | 0.868 |
| 4-Methyl-2-pentanone     | Pentanitrile             | 1.394            | 1.395 | 0.797         | 0.795 |
| 4-Methyl-2-pentanone     | 1-Butanol                | 1.394            | 1.397 | 0.797         | 0.812 |
| 2-Methyl-1-propanol      | Pentanitrile             | 1.394            | 1.395 | 0.798         | 0.795 |
| 2-Methyl-1-propanol      | 2-Hexanone               | 1.394            | 1.395 | 0.798         | 0.810 |
| 2-Butanol                | 2,4-Dimethyl-3-pentanone | 1.395            | 1.399 | 0.803         | 0.805 |
| 2-Hexanone               | 1-Butanol                | 1.395            | 1.397 | 0.810         | 0.812 |
| Pentanitrile             | 2,4-Dimethyl-3-pentanone | 1.395            | 1.399 | 0.795         | 0.805 |
| 2-Chlorobutane           | Isobutyl butyrate        | 1.395            | 1.399 | 0.868         | 0.860 |
| Butyric acid             | 2-Methoxyethanol         | 1.396            | 1.400 | 0.955         | 0.960 |
| 1-Butanol                | 3-Methyl-2-pentanone     | 1.397            | 1.398 | 0.812         | 0.808 |
| 1-Chloro-2-methylpropane | Isobutyl butyrate        | 1.397            | 1.399 | 0.872         | 0.860 |
| 1-Chloro-2-methylpropane | Pentyl acetate           | 1.397            | 1.400 | 0.872         | 0.871 |
| Methyl methacrylate      | 3-Methyl-2-pentanone     | 1.398            | 1.398 | 0.795         | 0.808 |
| Triethylamine            | 2,2,3-Trimethylpentane   | 1.399            | 1.401 | 0.723         | 0.712 |
| Butylamine               | Dodecane                 | 1.399            | 1.400 | 0.736         | 0.746 |
| Isobutyl butyrate        | 1-Chlorobutane           | 1.399            | 1.401 | 0.860         | 0.875 |
| 1-Nitropropane           | Propionic anhydride      | 1.399            | 1.400 | 0.995         | 1.007 |
| Pentyl acetate           | 1-Chlorobutane           | 1.400            | 1.400 | 0.871         | 0.881 |
| Pentyl acetate           | Tetrahydrofuran          | 1.400            | 1.404 | 0.871         | 0.885 |
| Dodecane                 | Dipropylamine            | 1.400            | 1.400 | 0.746         | 0.736 |
| 1-Chlorobutane           | Tetrahydrofuran          | 1.401            | 1.404 | 0.871         | 0.885 |
| Isopentanoic acid        | 2-Ethoxyethanol          | 1.402            | 1.405 | 0.923         | 0.926 |
| Dipropylamine            | Cyclopentane             | 1.403            | 1.404 | 0.736         | 0.740 |
| 2-Pentanol               | 4-Heptanone              | 1.404            | 1.405 | 0.804         | 0.813 |
| 3-Methyl-1-butanol       | Hexanonitrile            | 1.404            | 1.405 | 0.805         | 0.801 |
| 3-Methyl-1-butanol       | 4-Heptanone              | 1.404            | 1.405 | 0.805         | 0.813 |
| Hexanonitrile            | 4-Heptanone              | 1.405            | 1.405 | 0.801         | 0.813 |
| Hexanonitrile            | 1-Pentanol               | 1.405            | 1.408 | 0.801         | 0.810 |
| Hexanonitrile            | 2-Methyl-1-butanol       | 1.405            | 1.409 | 0.801         | 0.815 |
| 4-Heptanone              | 1-Pentanol               | 1.405            | 1.408 | 0.813         | 0.810 |

**TABLE 11.12** Solvents Having the Same Refractive Index and the Same Density at 25°C (*Continued*)

| Solvent 1                          | Solvent 2                          | Refractive index |       | Density, g/mL |       |
|------------------------------------|------------------------------------|------------------|-------|---------------|-------|
|                                    |                                    | 1                | 2     | 1             | 2     |
| 2-Ethoxyethanol                    | Pentanoic acid                     | 1.405            | 1.406 | 0.926         | 0.936 |
| 2-Heptanone                        | 1-Pentanol                         | 1.406            | 1.408 | 0.811         | 0.810 |
| 2-Heptanone                        | 2-Methyl-1-butanol                 | 1.406            | 1.409 | 0.811         | 0.815 |
| 2-Heptanone                        | Dipentyl ether                     | 1.406            | 1.410 | 0.811         | 0.799 |
| 2-Pentanol                         | 3-Isopropyl-2-pentanone            | 1.407            | 1.409 | 0.804         | 0.808 |
| 1-Pentanol                         | Dipentyl ether                     | 1.408            | 1.410 | 0.810         | 0.799 |
| 2-Methyl-1-butanol                 | Dipentyl ether                     | 1.409            | 1.410 | 0.815         | 0.799 |
| Isopentyl isopentanoate            | Allyl alcohol                      | 1.410            | 1.411 | 0.853         | 0.847 |
| Dipentyl ether                     | 2-Octanone                         | 1.410            | 1.414 | 0.799         | 0.814 |
| 2,4-Dimethyldioxane                | 3-Chloropentene                    | 1.412            | 1.413 | 0.935         | 0.932 |
| 2,4-Dimethyldioxane                | Hexanoic acid                      | 1.412            | 1.415 | 0.935         | 0.923 |
| Diethyl malonate                   | Ethyl cyanoacetate                 | 1.412            | 1.415 | 1.051         | 1.056 |
| 3-Chloropentene                    | Octanoic acid                      | 1.413            | 1.415 | 0.932         | 0.923 |
| 2-Octanone                         | 1-Hexanol                          | 1.414            | 1.416 | 0.814         | 0.814 |
| 2-Octanone                         | Octanonitrile                      | 1.414            | 1.418 | 0.814         | 0.810 |
| 3-Octanone                         | 3-Methyl-2-heptanone               | 1.414            | 1.416 | 0.830         | 0.818 |
| 3-Methyl-2-heptanone               | 1-Hexanol                          | 1.415            | 1.416 | 0.818         | 0.814 |
| 3-Methyl-2-heptanone               | Octanonitrile                      | 1.415            | 1.418 | 0.818         | 0.810 |
| 1-Hexanol                          | Octanonitrile                      | 1.416            | 1.418 | 0.814         | 0.810 |
| Dibutylamine                       | Allylamine                         | 1.416            | 1.419 | 0.756         | 0.758 |
| Allylamine                         | Methylcyclohexane                  | 1.419            | 1.421 | 0.758         | 0.765 |
| Butyrolactone                      | 1,3-Propanediol                    | 1.434            | 1.438 | 1.051         | 1.049 |
| Butyrolactone                      | Diethyl maleate                    | 1.434            | 1.438 | 1.051         | 1.064 |
| 2-Chloromethyl-2-propanol          | Diethyl maleate                    | 1.436            | 1.438 | 1.059         | 1.064 |
| N-Methylmorpholine                 | Dibutyl decanedioate               | 1.436            | 1.440 | 0.924         | 0.932 |
| 1,3-Propanediol                    | Diethyl maleate                    | 1.438            | 1.438 | 1.049         | 1.064 |
| Methyl salicylate                  | Diethyl sulfide                    | 1.438            | 1.442 | 0.836         | 0.831 |
| Methyl salicylate                  | 1-Butanethiol                      | 1.438            | 1.442 | 0.836         | 0.837 |
| 1-Chlorodecane                     | Mesityl oxide                      | 1.441            | 1.442 | 0.862         | 0.850 |
| Diethylene glycol                  | Formamide                          | 1.445            | 1.446 | 1.128         | 1.129 |
| Diethylene glycol                  | Ethylene glycol diglycidyl ether   | 1.445            | 1.447 | 1.128         | 1.134 |
| Formamide                          | Ethylene glycol diglycidyl ether   | 1.446            | 1.447 | 1.129         | 1.134 |
| 2-Methylmorpholine                 | Cyclohexanone                      | 1.446            | 1.448 | 0.951         | 0.943 |
| 2-Methylmorpholine                 | 1-Amino-2-propanol                 | 1.446            | 1.448 | 0.951         | 0.961 |
| Dipropylene glycol monoethyl ether | Tetrahydrofurfuryl alcohol         | 1.446            | 1.450 | 1.043         | 1.050 |
| 1-Amino-2-methyl-2-pentanol        | 2-Butylcyclohexanone               | 1.449            | 1.453 | 0.904         | 0.901 |
| 2-Propylcyclohexanone              | 4-Methylcyclohexanol               | 1.452            | 1.454 | 0.923         | 0.908 |
| Carbon tetrachloride               | 4,5-Dichloro-1,3-dioxolane-2-one   | 1.459            | 1.461 | 1.584         | 1.591 |
| N-Butyldiethanolamine              | Cyclohexanol                       | 1.461            | 1.465 | 0.965         | 0.968 |
| D- $\alpha$ -Pinene                | <i>trans</i> -Decahydronaphthalene | 1.464            | 1.468 | 0.855         | 0.867 |
| Propylbenzene                      | <i>p</i> -Xylene                   | 1.490            | 1.493 | 0.858         | 0.857 |
| Propylbenzene                      | Toluene                            | 1.490            | 1.494 | 0.858         | 0.860 |

**TABLE 11.12** Solvents Having the Same Refractive Index and the Same Density at 25°C (*Continued*)

| Solvent 1                    | Solvent 2                  | Refractive index |       | Density, g/mL |       |
|------------------------------|----------------------------|------------------|-------|---------------|-------|
|                              |                            | 1                | 2     | 1             | 2     |
| Phenyl 1-hydroxyphenyl ether | 1,3-Dimorpholyl-2-propanol | 1.491            | 1.493 | 1.081         | 1.094 |
| Phenetole                    | Pyridine                   | 1.505            | 1.507 | 0.961         | 0.978 |
| 2-Furanmethanol              | Thiophene                  | 1.524            | 1.526 | 1.057         | 1.059 |
| <i>m</i> -Cresol             | Benzaldehyde               | 1.542            | 1.544 | 1.037         | 1.041 |

**TABLE 11.13** McReynolds’ Constants for Stationary Phases in Gas Chromatography

| Stationary phase                                                                       | Chemical type                           | Similar stationary phases     | Temp., °C |     | McReynolds' constants |     |     |     |     |     | USP code |
|----------------------------------------------------------------------------------------|-----------------------------------------|-------------------------------|-----------|-----|-----------------------|-----|-----|-----|-----|-----|----------|
|                                                                                        |                                         |                               | Min       | Max | x'                    | y'  | z'  | u'  | s'  | Σ   |          |
| Boiling-point separation of broad molecular weight range of compounds; nonpolar phases |                                         |                               |           |     |                       |     |     |     |     |     |          |
| Squalane                                                                               | 2,6,10,15,19,23-Hexamethyltetracosane   |                               | 20        | 150 | 0                     | 0   | 0   | 0   | 0   | 0   |          |
| Paraffin oil                                                                           |                                         |                               |           |     | 9                     | 5   | 2   | 6   | 11  | 33  |          |
| Apiezon® L                                                                             |                                         |                               | 50        | 300 | 32                    | 22  | 15  | 32  | 42  | 143 |          |
| SPB-1                                                                                  | Poly(dimethylsiloxane)                  | SA-1, DB-1                    | −60       | 320 | 4                     | 58  | 43  | 56  | 38  | 199 |          |
| SP™ -2100                                                                              | Poly(dimethylsiloxane)                  | DC-200, SE 30, UC W98, DC 200 | 0         | 350 | 17                    | 57  | 45  | 67  | 43  | 229 | G 9      |
| OV-1                                                                                   | Methylsiloxane gum                      |                               | 100       | 350 | 16                    | 55  | 44  | 65  | 42  | 227 | G 2      |
| OV-101                                                                                 | Methylsiloxane fluid                    |                               | 20        | 350 | 17                    | 57  | 45  | 67  | 43  | 234 | G 1      |
| SPB-5                                                                                  | 1% Vinyl, 5% phenyl methyl polysiloxane | SA-5, DB-5                    | −60       | 320 | 19                    | 74  | 64  | 93  | 62  | 312 |          |
| SE-54                                                                                  | 1% Vinyl, 5% phenyl methyl polysiloxane | PTE-5                         | 50        | 300 | 19                    | 74  | 64  | 93  | 62  | 312 | G 36     |
| SE-52                                                                                  | 5% Phenyl methyl polysiloxane           |                               | 50        | 300 | 32                    | 72  | 65  | 98  | 67  | 334 | G 27     |
| OV-73                                                                                  | 5.5% Phenyl methyl polysiloxane         | SP-400                        | 0         | 325 | 40                    | 86  | 76  | 114 | 85  | 401 | G 27     |
| OV-3                                                                                   | Poly(dimethyldiphenylsiloxane); 90%:10% |                               | 0         | 350 | 44                    | 86  | 81  | 124 | 88  | 423 |          |
| Dexsil® 300                                                                            | Carborane—methyl silicone               |                               | 50        | 450 | 47                    | 80  | 103 | 148 | 96  | 474 | G 33     |
| Dexsil® 400                                                                            | Carborane—methyl-phenyl silicone        |                               | 50        | 400 | 72                    | 108 | 118 | 166 | 123 | 587 |          |



**TABLE 11.13** McReynolds' Constants for Stationary Phases in Gas Chromatography (*Continued*)

| Stationary phase                                                                                            | Chemical type                           | Similar stationary phases  | Temp., °C |     | McReynolds' constants |           |           |           |           |      | USP code |
|-------------------------------------------------------------------------------------------------------------|-----------------------------------------|----------------------------|-----------|-----|-----------------------|-----------|-----------|-----------|-----------|------|----------|
|                                                                                                             |                                         |                            | Min       | Max | <i>x'</i>             | <i>y'</i> | <i>z'</i> | <i>u'</i> | <i>s'</i> | Σ    |          |
| Boiling-point separation of broad molecular weight range of compounds; nonpolar phases ( <i>continued</i> ) |                                         |                            |           |     |                       |           |           |           |           |      |          |
| OV-7                                                                                                        | 20% Phenyl methyl polysiloxane          | DC 550                     | 0         | 350 | 69                    | 113       | 111       | 171       | 128       | 592  |          |
| SPB-20                                                                                                      | 20% Phenyl methyl polysiloxane          | SPB-35, SPB-1701, DB-1301  | <20       | 300 | 67                    | 116       | 117       | 174       | 131       | 605  |          |
| Di-(2-ethylhexyl)-sebacate                                                                                  |                                         |                            | −20       | 125 | 72                    | 168       | 108       | 180       | 125       | 653  | G 11     |
| DC 550                                                                                                      | 25% Phenyl methyl polysiloxane          |                            | 20        | 225 | 81                    | 124       | 124       | 189       | 145       | 663  | G 28     |
| Unsaturated hydrocarbons and other compounds of intermediate polarity                                       |                                         |                            |           |     |                       |           |           |           |           |      |          |
| Diisodecyl phthalate                                                                                        |                                         |                            | 20        | 150 | 84                    | 173       | 137       | 218       | 155       | 767  | G 24     |
| OV-11                                                                                                       | 35% Phenyl methyl polysiloxane          |                            | 0         | 350 | 102                   | 142       | 145       | 219       | 178       | 786  |          |
| OV-1701                                                                                                     | Vinyl methyl poly-siloxane              | SPB-1701, SA-1701, DB-1701 | 0         | 250 | 67                    | 170       | 152       | 228       | 171       | 789  |          |
| Poly-I 110                                                                                                  |                                         |                            |           | 275 | 115                   | 194       | 122       | 204       | 202       | 837  | G 37     |
| SP-2250                                                                                                     | Poly(phenylmethyl-siloxane); 50% phenyl | OV-17, DB-17               | 0         | 375 | 119                   | 158       | 162       | 243       | 202       | 884  | G 3      |
| Dexsil® 410                                                                                                 | Carborane—methylcyano ethyl silicone    |                            | 50        | 400 | 72                    | 286       | 174       | 249       | 171       | 952  |          |
| UCON® LB-550-X                                                                                              | Polyalkylene glycol                     |                            | 20        | 200 | 118                   | 271       | 158       | 243       | 206       | 996  |          |
| UCON LB-1880-X                                                                                              | Polyalkylene glycol                     |                            |           | 200 | 123                   | 275       | 161       | 249       | 212       | 1020 | G 18     |
| Poly-A 103                                                                                                  |                                         |                            |           | 275 | 115                   | 331       | 144       | 263       | 214       | 1072 | G 10     |

**TABLE 11.13** McReynolds' Constants for Stationary Phases in Gas Chromatography (*Continued*)

| Stationary phase                                                      | Chemical type                                  | Similar stationary phases | Temp., °C |     | McReynolds' constants |           |           |           |           |      | USP code |
|-----------------------------------------------------------------------|------------------------------------------------|---------------------------|-----------|-----|-----------------------|-----------|-----------|-----------|-----------|------|----------|
|                                                                       |                                                |                           | Min       | Max | <i>x'</i>             | <i>y'</i> | <i>z'</i> | <i>u'</i> | <i>s'</i> | Σ    |          |
| Unsaturated hydrocarbons and other compounds of intermediate polarity |                                                |                           |           |     | (continued)           |           |           |           |           |      |          |
| OV-22                                                                 | Poly(diphenyldimethylsiloxane); 65%:35%        |                           | 0         | 350 | 160                   | 188       | 191       | 283       | 253       | 1075 |          |
| Di(2-ethylhexyl) phthalate                                            |                                                |                           |           | 150 | 135                   | 254       | 213       | 320       | 235       | 1157 | G 22     |
| OV-25                                                                 | Poly(diphenyldimethylsiloxane); 75%:25%        |                           | 0         | 350 | 178                   | 204       | 208       | 305       | 280       | 1175 | G 17     |
| Moderately polar compounds                                            |                                                |                           |           |     |                       |           |           |           |           |      |          |
| DC QF-1                                                               |                                                |                           | 0         | 250 | 144                   | 233       | 355       | 463       | 305       | 1500 |          |
| OV-210                                                                | 50% Trifluoropropylmethylpolysiloxane          | SP-2401, DB-210           | 0         | 275 | 146                   | 238       | 358       | 468       | 310       | 1520 | G 6      |
| OV-215                                                                | Poly(trifluoropropylmethylsiloxane)            |                           | 0         | 275 | 149                   | 240       | 363       | 478       | 315       | 1545 |          |
| UCON-50-HB-2000                                                       | Polyalkylene glycol                            |                           | 0         | 200 | 202                   | 394       | 253       | 392       | 341       | 1582 |          |
| Triton® X-100                                                         | Octylphenoxy polyethoxy ethanol                |                           | 0         | 190 | 203                   | 399       | 268       | 402       | 362       | 1634 |          |
| UCON 50-HB-5100                                                       | Polyglycol                                     |                           | 0         | 200 | 214                   | 418       | 278       | 421       | 375       | 1706 |          |
| XE-60                                                                 | Poly(cyanoethylphenylmethylsiloxane)           |                           | 0         | 250 | 204                   | 381       | 340       | 493       | 367       | 1785 | G 26     |
| OV-225                                                                | 25% Cyanopropyl 25% phenyl methyl polysiloxane | DB-225, DB-23             | 0         | 265 | 228                   | 369       | 338       | 492       | 386       | 1813 | G 19     |
| Ipegal CO-880                                                         | Nonylphenoxypoly(ethyleneoxy)ethanol           |                           | 100       | 200 | 259                   | 461       | 311       | 482       | 426       | 1939 | G 31     |
| Triton® X-305                                                         | Octylphenoxy polyethoxy ethanol                |                           | 200       | 250 | 262                   | 467       | 314       | 488       | 430       | 1961 |          |

**TABLE 11.13** McReynolds' Constants for Stationary Phases in Gas Chromatography (*Continued*)

| Stationary phase    | Chemical type                               | Similar stationary phases | Temp., °C |     | McReynolds' constants |           |           |           |           |      | USP code |
|---------------------|---------------------------------------------|---------------------------|-----------|-----|-----------------------|-----------|-----------|-----------|-----------|------|----------|
|                     |                                             |                           | Min       | Max | <i>x'</i>             | <i>y'</i> | <i>z'</i> | <i>u'</i> | <i>s'</i> | Σ    |          |
| Polar compounds     |                                             |                           |           |     |                       |           |           |           |           |      |          |
| Hi-EFF-3BP          | Neopentylglycol succinate                   | DB-WAX, SA-WAX            | 50        | 230 | 272                   | 469       | 366       | 539       | 474       | 2120 | G 21     |
| Carbowax 20M-TPA    | Polyethyleneglycol + terephthalic acid      |                           | 60        | 250 | 321                   | 367       | 368       | 573       | 520       | 2149 | G 25     |
| Supelcowax™ 10      | Polyethyleneglycol + terephthalic acid      |                           | 50        | 280 | 305                   | 551       | 360       | 562       | 484       | 2262 |          |
| SP-1000             | Polyethyleneglycol + terephthalic acid      |                           | 60        | 220 | 304                   | 552       | 359       | 549       | 498       | 2262 |          |
| Carbowax 20M Nukol™ | Polyethyleneglycol                          | SP-2300                   | 25        | 275 | 322                   | 536       | 368       | 572       | 510       | 2308 | G 16     |
|                     |                                             | SP-1000, FFAP, OV-351     |           |     | 311                   | 572       | 374       | 572       | 520       | 2349 |          |
| Carbowax 3350       |                                             | Formerly Carbowax 4000    | 60        | 200 | 325                   | 551       | 375       | 582       | 520       | 2353 | G 15     |
| OV-351              | Polyethyleneglycol + nitroterephthalic acid | SP-1000                   | 50        | 270 | 335                   | 552       | 382       | 583       | 540       | 2392 |          |
| SP-2300             | 36% Cyanopropyl                             |                           | 25        | 275 | 316                   | 495       | 446       | 637       | 530       | 2424 |          |
| Silar 5 CP          | 50% Cyanopropyl phenyl silicone             | SP-2300                   | 0         | 250 | 319                   | 495       | 446       | 637       | 531       | 2428 | G 7      |

**TABLE 11.13** McReynolds' Constants for Stationary Phases in Gas Chromatography (*Continued*)

| Stationary phase                                           | Chemical type                  | Similar stationary phases | Temp., °C     |     | McReynolds' constants |                |     |     |     |      | USP code |
|------------------------------------------------------------|--------------------------------|---------------------------|---------------|-----|-----------------------|----------------|-----|-----|-----|------|----------|
|                                                            |                                |                           | Min           | Max | x'                    | y'             | z'  | u'  | s'  | Σ    |          |
| Polar compounds                                            |                                |                           |               |     |                       |                |     |     |     |      |          |
| FFAP                                                       | Phenyldiethanolamine succinate |                           | 50            | 250 | 340                   | 580            | 397 | 602 | 627 | 2546 | G 35     |
| Hi-EFF-10BP                                                |                                |                           | 20            | 230 | 386                   | 555            | 472 | 674 | 656 | 2744 | G 21     |
| Carbowax 1450                                              |                                |                           | Formerly 1540 | 50  | 175                   | 371            | 639 | 453 | 666 | 641  | 2770     |
| SP-2380                                                    | 55% Cyanopropyl                | Silar 7 CP                | 25            | 275 | 402                   | 629            | 520 | 744 | 623 | 2918 |          |
| SP-2310                                                    |                                |                           |               |     | 440                   | 637            | 605 | 840 | 670 | 3192 |          |
| SP-2330                                                    |                                |                           |               |     | 68% Cyanopropyl       | SP-2331, SH-60 | 25  | 275 | 490 | 725  | 630      |
| Silar 9 CP                                                 | 90% Cyanopropyl phenyl         |                           | 50            | 250 | 489                   | 725            | 631 | 913 | 778 | 3536 | G 8      |
| Hi-EFF-1BP                                                 | Diethyleneglycol succinate     |                           | 20            | 200 | 499                   | 751            | 593 | 840 | 860 | 3543 | G 4      |
| SP-2340                                                    | 75% Cyanopropyl phenyl         | OV-275, SH-80             | <25           | 275 | 520                   | 757            | 659 | 942 | 800 | 3678 |          |
| Silar 10 CP                                                | 100% Cyanopropyl silicone      | SP-2340                   | 25            | 275 | 523                   | 757            | 659 | 942 | 801 | 3682 | G 5      |
| THEED                                                      | Amino alcohol                  |                           | 0             | 125 | 463                   | 942            | 626 | 801 | 893 | 3725 |          |
| OV-275                                                     | Dicyanoallylsilicone           |                           | 25            | 250 | 629                   | 872            | 763 | 110 | 849 | 4219 |          |
| Absolute index values on squalane for reference compounds: |                                |                           |               | 653 | 590                   | 627            | 652 |     | 699 |      |          |

**Note:** USP code is the United States Pharmacopeia designation.

11.4.1 McReynolds' Constants

The *Kovats retention indices* (R.I.) indicate where compounds will appear on a chromatogram with respect to unbranched alkanes injected with the sample. By definition, the R.I. for pentane is 500, for hexane is 600, for heptane is 700, and so on, regardless of the column used or the operating conditions, although the exact conditions and column must be specified, such as liquid loading, particular support used, and any pretreatment. For example, suppose that on a 20% squalane column at 100°C, the retention times for hexane, benzene, and octane are found to be 15, 16, and 25 min, respectively. On a graph of  $\ln t'_R$  (napierian logarithm of the adjusted retention time) of the alkanes versus their retention indices, a R.I. of 653 for benzene is read off the graph. The number 653 for benzene (see last line of Table 11.13 in the column headed “1” under “Reference compounds”) means that it elutes halfway between hexane and heptane on a logarithmic time scale. If the experiment is repeated with a dinonyl phthalate column, the R.I. for benzene is found to be 736 (lying between heptane and octane), which implies that dinonyl phthalate will retard benzene slightly more than squalane will; that is, dinonyl phthalate is slightly more polar than squalane by  $\Delta I = 83$  units (the entry in Table 11.13 for dinonyl phthalate in the column headed “1” under “Reference compounds”). The difference gives a measure of solute-solvent interaction due to all intermolecular forces other than London dispersion forces. The latter are the principal solute-solvent effects with squalane.

TABLE 11.14 Characteristics of Selected Supercritical Fluids

| Fluid                  | Critical<br>temperature, K (°C) | Critical<br>pressure, atm (psi) |
|------------------------|---------------------------------|---------------------------------|
| Ammonia                | 406 (133)                       | 111.3 (1636)                    |
| Argon                  | 151 (– 122)                     | 48.1 (707)                      |
| Benzene                | 562 (289)                       | 48.3 (710)                      |
| Butane                 | 425 (125)                       | 37.5 (551)                      |
| Carbon dioxide         | 304 (31)                        | 72.8 (1070)                     |
| Carbon disulfide       | 552 (279)                       | 78.0 (1147)                     |
| Chlorotrifluoromethane | 379 (106)                       | 40 (588)                        |
| 2,2-Dimethylpropane    | 434 (161)                       | 31.6 (464)                      |
| Ethane                 | 305 (32)                        | 48.2 (706)                      |
| Fluoromethane          | 318 (45)                        | 58.0 (853)                      |
| Heptane                | 540 (267)                       | 27.0 (397)                      |
| Hexane                 | 507 (234)                       | 29.3 (431)                      |
| Hydrogen sulfide       | 373 (100)                       | 88.2 (1296)                     |
| Krypton                | 209 (– 64)                      | 54.3 (798)                      |
| Methane                | 191 (– 82)                      | 45.4 (667)                      |
| Methanol               | 513 (240)                       | 79.9 (1175)                     |
| 2-Methylpropane        | 408 (65)                        | 36.0 (529)                      |
| Nitrogen               | 126 (– 147)                     | 33.5 (492)                      |
| Nitrogen(I) oxide      | 310 (37)                        | 71.5 (1051)                     |
| Pentane                | 470 (197)                       | 33.3 (490)                      |
| Propane                | 470 (197)                       | 41.9 (616)                      |
| Sulfur dioxide         | 431 (158)                       | 77.8 (1144)                     |
| Sulfur hexafluoride    | 319 (46)                        | 37.1 (545)                      |
| Trichloromethane       | 536 (263)                       | 54.9 (807)                      |
| Trifluoromethane       | 299 (26)                        | 47.7 (701)                      |
| Water                  | 647 (374)                       | 217.6 (3199)                    |
| Xenon                  | 290 (17)                        | 57.6 (847)                      |

Now the overall effects due to hydrogen bonding, dipole moment, acid-base properties, and molecular configuration can be expressed as

$$\sum \Delta I = ax' + by' + cz' + du' + es'$$

where  $x' = \Delta I$  for benzene (the column headed "1" in Table 11.13, intermolecular forces typical of aromatics and olefins),  $y' = \Delta I$  for 1-butanol (the column headed "2" in Table 11.13, electron attraction typical of alcohols, nitriles, acids, and nitro and alkyl monochlorides, dichlorides and trichlorides),  $z' = \Delta I$  for 2-pentanone (the column headed "3" in Table 11.13, electron repulsion typical of ketones, ethers, aldehydes, esters, epoxides, and dimethylamino derivatives),  $u' = \Delta I$  for 1-nitropropane (the column headed "4" in Table 11.13, typical of nitro and nitrile derivatives), and  $s' = \Delta I$  for pyridine (or dioxane) (the column headed "5" in Table 11.13).

## 11.4.2 Chromatographic Behavior of Solutes

**11.4.2.1 Retention Behavior.** On a chromatogram the distance on the time axis from the point of sample injection to the peak of an eluted component is called the *uncorrected retention time*  $t_R$ . The corresponding retention volume is the product of retention time and flow rate, expressed as volume of mobile phase per unit time:

$$V_R = t_R F_c$$

The *average linear velocity*  $u$  of the mobile phase in terms of the column length  $L$  and the average linear velocity of eluent  $t_M$  (which is measured by the transit time of a nonretained solute) is

$$u = \frac{L}{t_M}$$

The *adjusted retention time*  $t'_R$  is given by

$$t'_R = t_R - t_M$$

When the mobile phase is a gas, a *compressibility factor*  $j$  must be applied to the adjusted retention volume to give the *net retention volume*:

$$V_N = jV_R$$

The compressibility factor is expressed by

$$j = \frac{3[(P_i/P_o)^2 - 1]}{2[(P_i/P_o)^3 - 1]}$$

where  $P_i$  is the carrier gas pressure at the column inlet and  $P_o$  that at the outlet.

**11.4.2.2 Partition Ratio.** The partition ratio is the additional time a solute band takes to elute, as compared with an unretained solute (for which  $k' = 0$ ), divided by the elution time of an unretained band:

$$k' = \frac{t_R - t_M}{t_M} = \frac{V_R - V_M}{V_M}$$

Retention time may be expressed as

$$t_R = t_M(1 + k') = \frac{L}{u}(1 + k')$$

**11.4.2.3 Relative Retention.** The relative retention  $\alpha$  of two solutes, where solute 1 elutes before solute 2, is given variously by

$$\alpha = \frac{k'_2}{k'_1} = \frac{V'_{R,2}}{V'_{R,1}} = \frac{t'_{R,2}}{t'_{R,1}}$$

The relative retention is dependent on (1) the nature of the stationary and mobile phases and (2) the column operating temperature.

**11.4.2.4 Column Efficiency.** Under ideal conditions the profile of a solute band resembles that given by a Gaussian distribution curve (Fig. 11.1). The efficiency of a chromatographic system is expressed by the effective plate number  $N_{\text{eff}}$ , defined from the chromatogram of a single band,

$$N_{\text{eff}} = \frac{L}{H} = 16 \left( \frac{t'_R}{W_b} \right)^2 = 5.54 \left( \frac{t'_R}{W_{1/2}} \right)^2$$

where  $L$  is the column length,  $H$  is the plate height,  $t'_R$  is the adjusted time for elution of the band center,  $W_b$  is the width at the base of the peak ( $W_b = 4\sigma$ ) as determined from the intersections of tangents to the inflection points with the baseline, and  $W_{1/2}$  is the width at half the peak height. Column efficiency, when expressed as the number of theoretical plates  $N_{\text{theor}}$  uses the uncorrected retention time in the foregoing expression. The two column efficiencies are related by

$$N_{\text{eff}} = N_{\text{theor}} \left( \frac{k'}{k' + 1} \right)^2$$

**11.4.2.5 Band Asymmetry.** The peak asymmetry factor  $AF$  is often defined as the ratio of peak half-widths at 10% of peak height, that is, the ratio  $b/a$ , as shown in Fig. 11.2. When the asymmetry ratio lies outside the range 0.95–1.15 for a peak of  $k' = 2$ , the effective plate number should be calculated from the expression

$$N = \frac{41.7(t'_R/W_{0.1})}{(a/b) + 1.25}$$

**11.4.2.6 Resolution.** The degree of separation or resolution,  $R_s$ , of two adjacent peaks is defined as the distance between band peaks (or centers) divided by the average bandwidth using  $W_b$ , as shown in Fig. 11.3.

$$R_s = \frac{t_{R,2} - t_{R,1}}{0.5(W_2 + W_1)}$$

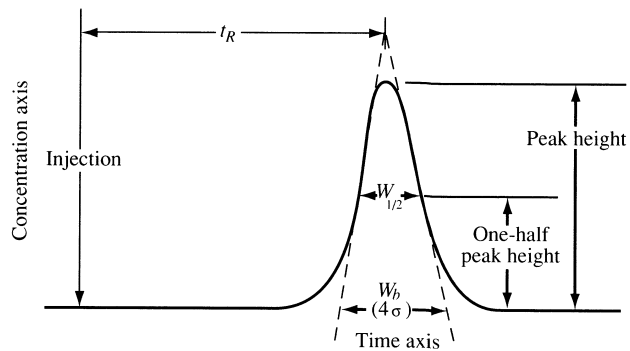
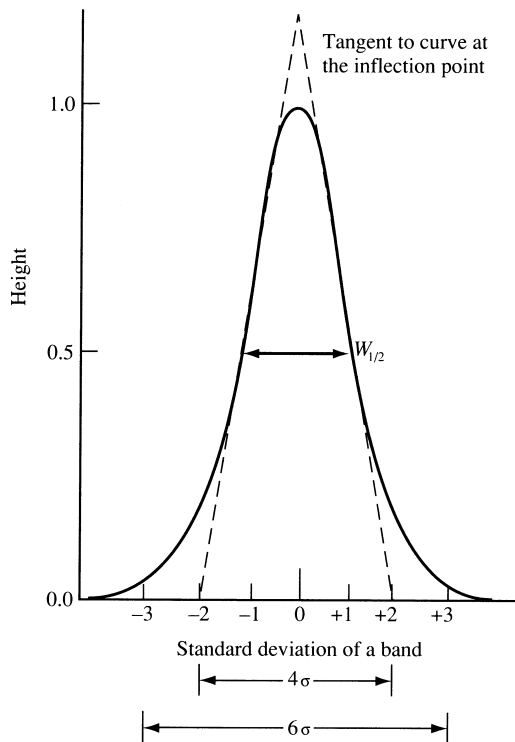


FIGURE 11.1 Profile of a solute band.



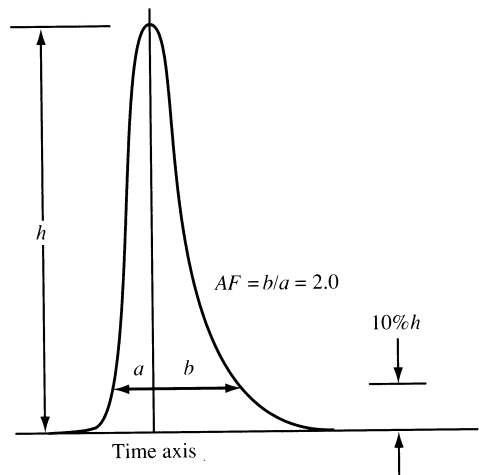


FIGURE 11.2 Band asymmetry.

For reasonable quantitative accuracy, peak maxima must be at least  $4\sigma$  apart. If so, then  $R_s = 1.0$ , which corresponds approximately to a 3% overlap of peak areas. A value of  $R_s = 1.5$  (for  $6\sigma$ ) represents essentially complete resolution with only 0.2% overlap of peak areas. These criteria pertain to roughly equal solute concentrations.

The fundamental resolution equation incorporates the terms involving the thermodynamics and kinetics of the chromatographic system:

$$R_s = \frac{1}{4} \left( \frac{\alpha - 1}{\alpha} \right) \left( \frac{k'}{1 + k'} \right) \left( \frac{L}{H} \right)^{1/2}$$

Three separate factors affect resolution: (1) a column selectivity factor that varies with  $\alpha$ , (2) a capacity factor that varies with  $k'$  (taken usually as  $k_2$ ), and (3) an efficiency factor that depends on the theoretical plate number.

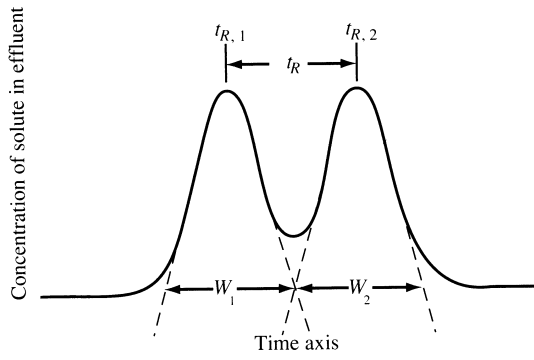


FIGURE 11.3 Definition of resolution.

**11.4.2.7 Time of Analysis.** The retention time required to perform a separation is given by

$$t_R = 16Rs^2 \left( \frac{\alpha}{\alpha - 1} \right)^2 \left[ \frac{(1 + k')^3}{(k')^2} \right] \left( \frac{H}{u} \right)$$

Now  $t_R$  is a minimum when  $k' = 2$ , that is, when  $t_R = 3t_M$ . There is little increase in analysis time when  $k'$  lies between 1 and 10. A twofold increase in the mobile-phase velocity roughly halves the analysis time (actually it is the ratio  $H/u$  which influences the analysis time). The ratio  $H/u$  can be obtained from the experimental plate height/velocity graph.

**11.4.2.8 High-Performance Liquid Chromatography.** Typical performances for various experimental conditions are given in Table 11.15. The data assume these reduced parameters:  $h = 3$ ,  $v = 4.5$ . The reduced plate height is

$$h = \frac{H}{d_p} = \frac{L}{Nd_p}$$

The reduced velocity of the eluent is

$$v = \frac{ud_p}{D_M} = \frac{Ld_p}{t_M D_M}$$

In these expressions,  $d_p$  is the particle diameter of the stationary phase that constitutes one plate height.  $D_M$  is the diffusion coefficient of the solute in the mobile phase.

**TABLE 11.15** Typical Performances in HPLC for Various Conditions

| Performances |           | Column parameters |                       |                 |
|--------------|-----------|-------------------|-----------------------|-----------------|
| $N$          | $t_M$ , s | $L$ , cm          | $d_p$ , $\mu\text{m}$ | $P$ , atm (psi) |
| 2 500        | 30        | 2.3               | 3                     | 18.4 (270)      |
| 2 500        | 30        | 3.7               | 5                     | 18.4 (270)      |
| 2 500        | 30        | 7.5               | 10                    | 18.4 (270)      |
| 5 000        | 30        | 4.5               | 3                     | 74 (1088)       |
| 5 000        | 30        | 7.5               | 5                     | 74 (1088)       |
| 5 000        | 30        | 15.0              | 10                    | 74 (1088)       |
| 10 000       | 30        | 9.0               | 3                     | 300 (4410)      |
| 10 000       | 30        | 15.0              | 5                     | 300 (4410)      |
| 10 000       | 30        | 30.0              | 10                    | 300 (4410)      |
| 10 000       | 30        | 9.0               | 3                     | 300 (4410)      |
| 10 000       | 60        | 9.0               | 3                     | 150 (2200)      |
| 10 000       | 90        | 9.0               | 3                     | 100 (1470)      |
| 15 000       | 90        | 2.3               | 3                     | 223 (3275)      |
| 15 000       | 120       | 2.3               | 3                     | 167 (2459)      |
| 11 100       | 30        | 10.0              | 3                     | 369 (5420)      |
| 11 100       | 37        | 10.0              | 3                     | 300 (4410)      |
| 11 100       | 101       | 10.0              | 3                     | 100 (1470)      |
| 27 800       | 231       | 25.0              | 3                     | 300 (4410)      |

Assumed reduced parameters:  $h = 3$ ,  $v = 4.5$ . These are optimum values from a graph of reduced plate height versus reduced linear velocity of the mobile phase.

### 11.4.3 Ion-Exchange (Normal Pressure, Columnar)

Ion-exchange methods are based essentially on a reversible exchange of ions between an external liquid phase and an ionic solid phase. The solid phase consists of a polymeric matrix, insoluble, but permeable, which contains fixed charge groups and mobile counter ions of opposite charge. These counter ions can be exchanged for other ions in the external liquid phase. Enrichment of one or several of the components is obtained if selective exchange forces are operative. The method is limited to substances at least partially in ionized form.

**11.4.3.1 Chemical Structure of Ion-Exchange Resins.** An ion-exchange resin usually consists of polystyrene copolymerized with divinylbenzene to build up an inert three-dimensional, cross-linked matrix of hydrocarbon chains. Protruding from the polymer chains are the ion-exchange sites distributed statistically throughout the entire resin particle. The ionic sites are balanced by an equivalent number of mobile counter ions. The type and strength of the exchanger is determined by these active groups. Ion-exchangers are designated anionic or cationic, according to whether they have an affinity for negative or positive counter ions. Each main group is further subdivided into strongly or weakly ionized groups. A selection of commercially available ion-exchange resins is given in Table 11.16.

The cross-linking of a polystyrene resin is expressed as the proportion by weight percent of divinylbenzene in the reaction mixture; for example, “×8” for 8 percent cross-linking. As the percentage is increased, the ionic groups come into effectively closer proximity, resulting in increased selectivity. Intermediate cross-linking, in the range of 4 to 8 percent, is usually used. An increase in cross-linking decreases the diffusion rate in the resin particles; the diffusion rate is the rate-controlling step in column operations. Decreasing the particle size reduces the time required for attaining equilibrium, but at the same time decreases the flow rate until it is prohibitively slow unless pressure is applied.

In most inorganic chromatography, resins of 100 to 200 mesh size are suitable; difficult separations may require 200 to 400 mesh resins. A flow rate of  $1 \text{ mL} \cdot \text{cm}^{-2} \cdot \text{min}^{-1}$  is often satisfactory. With HPLC columns, the flow rate in long columns of fine adsorbent can be increased by applying pressure.

**11.4.3.1.1 Macroreticular Resins.** Macroreticular resins are an agglomerate of randomly packed microspheres which extend through the agglomerate in a continuous non-gel pore structure. The channels throughout the rigid pore structure render the bead centers accessible even in non-aqueous solvents, in which microreticular resins do not swell sufficiently. Because of their high porosity and large pore diameters, these resins can handle large organic molecules.

**11.4.3.1.2 Microreticular Resins.** Microreticular resins, by contrast, are elastic gels that, in the dry state, avidly absorb water and other polar solvents in which they are immersed. While taking up solvent, the gel structure expands until the retractile stresses of the distended polymer network balance the osmotic effect. In nonpolar solvents, little or no swelling occurs and diffusion is impaired.

**11.4.3.1.3 Ion-Exchange Membranes.** Ion-exchange membranes are extremely flexible, strong membranes, composed of analytical grade ion-exchange resin beads (90%) permanently enmeshed in a poly(tetrafluoroethylene) membrane (10%). The membranes offer an alternative to column and batch methods, and can be used in many of the same applications as traditional ion exchange resins. Three ion-exchange resin types have been incorporated into membranes: AG 1-X8, AG 50W-X8, and Chelex 100.

### 11.4.3.2 Functional Groups

*Sulfonate exchangers* contain the group  $-\text{SO}_3^-$ , which is strongly acidic and completely dissociated whether in the H form or the cation form. These exchangers are used for cation exchange.

**TABLE 11.16** Guide to Ion-Exchange Resins

Dowex is the trade name of Dow resins; X (followed by a numeral) is percent cross-linked. Mesh size (dry) are available in the range 50 to 100, 100 to 200, 200 to 400, and sometimes minus 400.

S-DVB is the acronym for styrene-divinylbenzene.

MP is the acronym for macroporous resin. Mesh size (dry) is available in the range 20 to 50, 100 to 200, and 200 to 400.

Bio-Rex is the trade name for certain resins sold by Bio-Rad Laboratories.

Amberlite and Duolite are trade names of Rohm & Haas resins.

| Resin type and nominal percent cross-linkage                                    | Minimum wet capacity, mequiv $\cdot$ mL <sup>-1</sup> | Density (nominal), g $\cdot$ mL <sup>-1</sup> | Comments                                                                                                                                                                                    |
|---------------------------------------------------------------------------------|-------------------------------------------------------|-----------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Anion exchange resins—gel type—strongly basic—quaternary ammonium functionality |                                                       |                                               |                                                                                                                                                                                             |
| Dowex 1-X2                                                                      | 0.6                                                   | 0.65                                          | Strongly basic anion exchanger with S-DVB matrix for separation of small peptides, nucleotides, and large metal complexes. Molecular weight exclusion is <2700.                             |
| Dowex 1-X4                                                                      | 1.0                                                   | 0.70                                          | Strongly basic anion exchanger with S-DVB matrix for separation of organic acids, nucleotides, phosphoinositides, and other anions. Molecular weight exclusion is <1400.                    |
| Dowex 1-X8                                                                      | 1.2                                                   | 0.75                                          | Strongly basic anion exchanger with S-DVB matrix for separation of inorganic and organic anions with molecular weight exclusion <1000. 100–200 mesh is standard for analytical separations. |
| Dowex 2-X8                                                                      | 1.2                                                   | 0.75                                          | Strongly basic (but less basic than Dowex 1 type) anion exchanger with S-DVB matrix for deionization of carbohydrates and separation of sugars, sugar alcohols, and glycosides.             |
| Amberlite IRA-400                                                               | 1.4                                                   | 1.11                                          | 8% cross-linkage. Used for systems essentially free of organic materials.                                                                                                                   |
| Amberlite IRA-402                                                               | 1.3                                                   | 1.07                                          | Lower cross-linkage than IRA-400; better diffusion rate with large organic molecules.                                                                                                       |
| Amberlite IRA-410                                                               | 1.4                                                   | 1.12                                          | Dimethylethanolamine functionality and slightly lower basicity than IRA-400.                                                                                                                |
| Amberlite IRA-458                                                               | 1.2                                                   | 1.08                                          | Has an acrylic structure rather than S-DVB; hence more hydrophilic and resistant to organic fouling.                                                                                        |
| Anion exchange resin—gel type—intermediate basicity                             |                                                       |                                               |                                                                                                                                                                                             |
| Bio-Rex 5                                                                       | 2.8                                                   | 0.70                                          | Intermediate basic anion exchanger with primarily tertiary amines on a polyalkyle-neamine matrix for separation of organic acids.                                                           |

**TABLE 11.16** Guide to Ion-Exchange Resins (*Continued*)

| Resin type and nominal percent cross-linkage                                | Minimum wet capacity, mequiv $\cdot$ mL <sup>-1</sup> | Density (nominal), g $\cdot$ mL <sup>-1</sup> | Comments                                                                                                                                                                                                                                                                  |
|-----------------------------------------------------------------------------|-------------------------------------------------------|-----------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Anion exchange resins—gel type—weakly basic—polyamine functionality         |                                                       |                                               |                                                                                                                                                                                                                                                                           |
| Dowex 4-X4                                                                  | 1.6                                                   | 0.70                                          | Weakly basic anion exchanger with tertiary amines on an acrylic matrix for the deionization of carbohydrates. Use at pH <7.                                                                                                                                               |
| Amberlite IRA-68                                                            | 1.6                                                   | 1.06                                          | Acrylic-DVB with unusually high capacity for large organic molecules.                                                                                                                                                                                                     |
| Cation exchange resins—gel type—strongly acidic—sulfonic acid functionality |                                                       |                                               |                                                                                                                                                                                                                                                                           |
| Dowex 50W-X2                                                                | 0.6                                                   | 0.70                                          | Strongly acidic cation exchanger with S-DVB matrix for separation of peptides, nucleotides, and cations. Molecular weight exclusion <2700.                                                                                                                                |
| Dowex 50W-X4                                                                | 1.1                                                   | 0.80                                          | Strongly acidic cation exchanger with S-DVB matrix for separation of amino acids, nucleosides and cations. Molecular weight exclusion is <1400.                                                                                                                           |
| Dowex 50W-X8                                                                | 1.7                                                   | 0.80                                          | Strongly acidic cation exchanger with S-DVB matrix for separation of amino acids, metal cations, and cations. Molecular weight exclusion is <1000. 100–200 mesh is standard for analytical applications.                                                                  |
| Dowex 50W-X12                                                               | 2.1                                                   | 0.85                                          | Strongly acidic cation exchanger with S-DVB matrix used primarily for metal separations.                                                                                                                                                                                  |
| Dowex 50W-X16                                                               | 2.4                                                   | 0.85                                          | Strongly acidic cation exchanger with S-DVB matrix and high cross linkage.                                                                                                                                                                                                |
| Amberlite IR-120                                                            | 1.9                                                   | 1.26                                          | 8% styrene-DVB type; high physical stability.                                                                                                                                                                                                                             |
| Amberlite IR-122                                                            | 2.1                                                   | 1.32                                          | 10% styrene-DVB type; high physical stability and high capacity.                                                                                                                                                                                                          |
| Weakly acidic cation exchangers—gel type—carboxylic acid functionality      |                                                       |                                               |                                                                                                                                                                                                                                                                           |
| Duolite C-433                                                               | 4.5                                                   | 1.19                                          | Acrylic-DVB type; very high capacity. Used for metals removal and neutralization of alkaline solutions.                                                                                                                                                                   |
| Bio-Rex 70                                                                  | 2.4                                                   | 0.70                                          | Weakly acidic cation exchanger with carboxylate groups on a macroreticular acrylic matrix for separation and fractionation of proteins, peptides, enzymes, and amines, particularly high molecular weight solutes. Does not denature proteins as do styrene-based resins. |

**TABLE 11.16** Guide to Ion-Exchange Resins (*Continued*)

| Resin type and nominal percent cross-linkage                                         | Minimum wet capacity, mequiv · mL <sup>-1</sup> | Density (nominal), g · mL <sup>-1</sup> | Comments                                                                                                                                               |
|--------------------------------------------------------------------------------------|-------------------------------------------------|-----------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| Selective ion exchange resins                                                        |                                                 |                                         |                                                                                                                                                        |
| Duolite GT-73                                                                        | 1.3                                             | 1.30                                    | Removal of Ag, Cd, Cu, Hg, and Pb.                                                                                                                     |
| Amberlite IRA-743A                                                                   | 0.6                                             | 1.05                                    | Boron specific ion exchange resin.                                                                                                                     |
| Amberlite IRC-718                                                                    | 1.0                                             | 1.14                                    | Removal of transition metals.                                                                                                                          |
| Chelex® 100                                                                          | 0.4                                             | 0.65                                    | Weakly acidic chelating resin with S-DVB matrix for heavy metal concentration.                                                                         |
| Anion exchanger—macroreticular type—strongly basic—quaternary ammonium functionality |                                                 |                                         |                                                                                                                                                        |
| Amberlite IRA-910                                                                    | 1.1                                             | 1.09                                    | Dimethylethanolamine styrene-DVB type which offers slightly less silica removal than Amberlite IRA resin, but offers improved regeneration efficiency. |
| Amberlite IRA-938                                                                    | 0.5                                             | 1.20                                    | Pore size distribution between 2500 and 23 000 nm; suitable for removal of high molecular weight organic materials.                                    |
| Amberlite IRA-958                                                                    | 0.8                                             |                                         | Acrylic-DVB; resistant to organic fouling.                                                                                                             |
| AG MP-1                                                                              | 1.0                                             | 0.70                                    | Strongly basic macroporous anion exchanger with S-DVB matrix for separation of some enzymes, radioactive anions, and other applications.               |
| Cation exchange resin—macroreticular type—sulfonic acid functionality                |                                                 |                                         |                                                                                                                                                        |
| Amberlite 200                                                                        | 1.7                                             | 1.26                                    | Styrene-DVB with 20% DVB by weight; superior physical stability and greater resistance to oxidation by factor of three over comparable gel type resin. |
| AG MP-50                                                                             | 1.5                                             | 0.80                                    | Strongly acidic macroporous cation exchanger with S-DVB matrix for separation of radioactive cations and other applications.                           |
| Weak cation exchanger—macroreticular type—carboxylic acid or phenolic functionality  |                                                 |                                         |                                                                                                                                                        |
| Amberlite DP-1                                                                       | 2.5                                             | 1.17                                    | Methacrylic acid-DVB; high resin capacity. Use pH >5.                                                                                                  |
| Amberlite IRC-50                                                                     | 3.5                                             | 1.25                                    | Methacrylic acid-DVB. Selectivity adsorbs organic gases such as antibiotics, alkaloids, peptides, and amino acids. Use pH >5.                          |
| Duolite C-464                                                                        | 3.0                                             | 1.13                                    | Polyacrylic resin with high capacity and outstanding resistance to osmotic shock.                                                                      |

**TABLE 11.16** Guide to Ion-Exchange Resins (*Continued*)

| Resin type and nominal percent cross-linkage                                                             | Minimum wet capacity, mequiv · mL <sup>-1</sup> | Density (nominal), g · mL <sup>-1</sup> | Comments                                                                                                                                                                                     |
|----------------------------------------------------------------------------------------------------------|-------------------------------------------------|-----------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Weak cation exchanger—macroreticular type—carboxylic acid or phenolic functionality ( <i>continued</i> ) |                                                 |                                         |                                                                                                                                                                                              |
| Duolite A-7                                                                                              | 2.2                                             | 1.12                                    | Phenolic type resin. High porosity and hydrophilic matrix. pH range is 0 to 6.                                                                                                               |
| Duolite A-368                                                                                            | 1.7                                             | 1.04                                    | Styrene-DVB; pH range is 0 to 9.                                                                                                                                                             |
| Amberlite IRA-35                                                                                         | 1.1                                             |                                         | Acrylic-DVB; pH range is 0 to 9.                                                                                                                                                             |
| Amberlite IRA-93                                                                                         | 1.3                                             | 1.04                                    | Styrene-DVB; pH range is 0 to 9. Excellent resistance to oxidation and organic fouling.                                                                                                      |
| Liquid amines                                                                                            |                                                 |                                         |                                                                                                                                                                                              |
| Amberlite LA-1                                                                                           |                                                 |                                         | A secondary amine containing two highly branched aliphatic chains of M.W. 351 to 393. Solubility is 15 to 20 mg/mL in water. Used as 5 to 40% solutions in hydrocarbons.                     |
| Amberlite LA-2                                                                                           |                                                 |                                         | A secondary amine of M.W. 353 to 395. Insoluble in water.                                                                                                                                    |
| Microcrystalline exchanger                                                                               |                                                 |                                         |                                                                                                                                                                                              |
| AMP-1                                                                                                    | 4.0                                             |                                         | Microcrystalline ammonium molybdo-phosphate with cation exchange capacity of 1.2 mequiv/g. Selectively adsorbs larger alkali metal ions from smaller alkali metal ions, particularly cesium. |
| Ion retardation resin                                                                                    |                                                 |                                         |                                                                                                                                                                                              |
| AG 11 A8                                                                                                 |                                                 | 0.70                                    | Ion retardation resin containing paired anion (COO <sup>-</sup> ) and cation (CH <sub>3</sub> ) <sub>3</sub> N <sup>+</sup> sites. Selectively retards ionic substances.                     |

**Source:** J. A. Dean, ed., *Analytical Chemistry Handbook*, McGraw-Hill, New York, 1995.

*Carboxylate exchangers* contain —COOH groups which have weak acidic properties and will only function as cation exchangers when the pH is sufficiently high (pH > 6) to permit complete dissociation of the —COOH site. Outside this range the ion exchanger can be used only at the cost of reduced capacity.

*Quaternary ammonium exchangers* contain —R<sub>4</sub>N<sup>+</sup> groups which are strongly basic and completely dissociated in the OH form and the anion form.

*Tertiary amine exchangers* possess —R<sub>3</sub>NH<sub>2</sub> groups which have exchanging properties only in an acidic medium when a proton is bound to the nitrogen atom.

*Aminodiacetate exchangers* have the —N(CH<sub>2</sub>COOH)<sub>2</sub> group which has an unusually high preference for copper, iron, and other heavy metal cations and, to a lesser extent, for alkaline earth

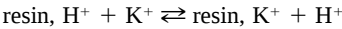
cations. The resin selectivity for divalent over monovalent ions is approximately 5000 to 1. The resin functions as a chelating resin at pH 4 and above. At very low pH, the resin acts as an anion exchanger. This exchanger is the column packing often used for ligand exchange.

**11.4.3.3 Ion-Exchange Equilibrium.** Retention differences among cations with an anion exchanger, or among anions with a cation exchanger, are governed by the physical properties of the solvated ions. The stationary phase will show these preferences:

1. The ion of higher charge.
2. The ion with the smaller solvated radius. Energy is needed to strip away the solvation shell surrounding ions with large hydrated radii, even though their crystallographic ionic radii may be less than the average pore opening in the resin matrix.
3. The ion that has the greater polarizability (which determines the Van der Waals' attraction).

To accomplish any separation of two cations (or two anions) of the same net charge, the stationary phase must show a preference for one more than the other. No variation in the eluant concentration will improve the separation. However, if the exchange involves ions of different net charges, the separation factor does depend on the eluant concentration. The more dilute the counterion concentration in the eluant, the more selective the exchange becomes for polyvalent ions.

In the case of an ionized resin, initially in the H-form and in contact with a solution containing  $K^+$  ions, an equilibrium exists:



which is characterized by the selectivity coefficient,  $k_{K/H}$ :

$$k_{K/H} = \frac{[K^+]_r [H^+]}{[H^+]_r [K^+]}$$

where the subscript  $r$  refers to the resin phase. Table 11.17 contains selectivity coefficients for cations and Table 11.18 for anions. Relative selectivities are of limited use for the prediction of the columnar

**TABLE 11.17** Relative Selectivity of Various Counter Cations

| Counterion                   | Relative selectivity for AG 50W-X8 resin | Counterion       | Relative selectivity for AG 50W-X8 resin |
|------------------------------|------------------------------------------|------------------|------------------------------------------|
| H <sup>+</sup>               | 1.0                                      | Zn <sup>2+</sup> | 2.7                                      |
| Li <sup>+</sup>              | 0.86                                     | Co <sup>2+</sup> | 2.8                                      |
| Na <sup>+</sup>              | 1.5                                      | Cu <sup>2+</sup> | 2.9                                      |
| NH <sub>4</sub> <sup>+</sup> | 1.95                                     | Cd <sup>2+</sup> | 2.95                                     |
| K <sup>+</sup>               | 2.5                                      | Ni <sup>2+</sup> | 3.0                                      |
| Rb <sup>+</sup>              | 2.6                                      | Ca <sup>2+</sup> | 3.9                                      |
| Cs <sup>+</sup>              | 2.7                                      | Sr <sup>2+</sup> | 4.95                                     |
| Cu <sup>+</sup>              | 5.3                                      | Hg <sup>2+</sup> | 7.2                                      |
| Ag <sup>+</sup>              | 7.6                                      | Pb <sup>2+</sup> | 7.5                                      |
| Tl <sup>+</sup>              | 10.7                                     | Ba <sup>2+</sup> | 8.7                                      |
| Mn <sup>2+</sup>             | 2.35                                     | Ce <sup>3+</sup> | 22                                       |
| Mg <sup>2+</sup>             | 2.5                                      | La <sup>3+</sup> | 22                                       |
| Fe <sup>2+</sup>             | 2.55                                     |                  |                                          |



TABLE 11.18 Relative Selectivity of Various Counter Anions

| Counterion                                  | Relative selectivity for Dowex 1-X8 resin | Relative selectivity for Dowex 2-X8 resin |
|---------------------------------------------|-------------------------------------------|-------------------------------------------|
| OH <sup>-</sup>                             | 1.0                                       | 1.0                                       |
| Benzenesulfonate <sup>-</sup>               | 500                                       | 75                                        |
| Salicylate <sup>-</sup>                     | 450                                       | 65                                        |
| Citrate                                     | 220                                       | 23                                        |
| I <sup>-</sup>                              | 175                                       | 17                                        |
| Phenate <sup>-</sup>                        | 110                                       | 27                                        |
| HSO <sub>4</sub> <sup>-</sup>               | 85                                        | 15                                        |
| ClO <sub>3</sub> <sup>-</sup>               | 74                                        | 12                                        |
| NO <sub>3</sub>                             | 65                                        | 8                                         |
| Br <sup>-</sup>                             | 50                                        | 6                                         |
| CN <sup>-</sup>                             | 28                                        | 3                                         |
| HSO <sub>3</sub> <sup>-</sup>               | 27                                        | 3                                         |
| BrO <sub>3</sub> <sup>-</sup>               | 27                                        | 3                                         |
| NO <sub>2</sub>                             | 24                                        | 3                                         |
| Cl <sup>-</sup>                             | 22                                        | 2.3                                       |
| ClO <sub>4</sub> <sup>-</sup>               | 20                                        |                                           |
| SCN <sup>-</sup>                            | 8.0                                       |                                           |
| HCO <sub>3</sub> <sup>-</sup>               | 6.0                                       | 1.2                                       |
| IO <sub>3</sub> <sup>-</sup>                | 5.5                                       | 0.5                                       |
| H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> | 5.0                                       | 0.5                                       |
| Formate <sup>-</sup>                        | 4.6                                       | 0.5                                       |
| Acetate <sup>-</sup>                        | 3.2                                       | 0.5                                       |
| Propanoate <sup>-</sup>                     | 2.6                                       | 0.3                                       |
| F <sup>-</sup>                              | 1.6                                       | 0.3                                       |

exchange behavior of a cation because they do not take account of the influence of the aqueous phase. More specific information about the behavior to be expected from a cation in a column elution experiment is given by the equilibrium distribution coefficient  $K_d$ .

The partitioning of the potassium ion between the resin and solution phases is described by the concentration distribution ratio,  $D_c$ :

$$(D_c)_K = \frac{[K^+]_r}{[K^+]}$$

Combining the equations for the selectivity coefficient and for  $D_c$ :

$$(D_c)_K = k_{K/H} \frac{[H^+]_r}{[H^+]}$$

The foregoing equation reveals that essentially the concentration distribution ratio for trace concentrations of an exchanging ion is independent of the respective solution of that ion and that the uptake of each trace ion by the resin is directly proportional to its solution concentration. However, the

concentration distribution ratios are inversely proportional to the solution concentration of the resin counterion.

To accomplish any separation of two cations (or two anions), one of these ions must be taken up by the resin in distinct preference to the other. This preference is expressed by the separation factor (or relative retention),  $\alpha_{K/Na}$ , using  $K^+$  and  $Na^+$  as the example:

$$\alpha_{K/Na} = \frac{(D_c)_K}{(D_c)_{Na}} = \frac{k_{K/H}}{k_{Na/H}} = K_{K/Na}$$

The more  $\alpha$  deviates from unity for a given pair of ions, the easier it will be to separate them. If the selectivity coefficient is unfavorable for the separation of two ions of the same charge, no variation in the concentration of  $H^+$  (the eluant) will improve the separation.

The situation is entirely different if the exchange involves ions of different net charges. Now the separation factor does depend on the eluant concentration. For example, the more dilute the counterion concentration in the eluant, the more selective the exchange becomes for the ion of higher charge.

In practice, it is more convenient to predict the behavior of an ion, for any chosen set of conditions, by employing a much simpler distribution coefficient,  $D_g$ , which is defined as the concentration of a solute in the resin phase divided by its concentration in the liquid phase, or:

$$D_g = \frac{\text{concentration of solute, resin phase}}{\text{concentration of solute, liquid phase}}$$

$$D_g = \frac{\% \text{ solute within exchanger}}{\% \text{ solute within solution}} \times \frac{\text{volume of solution}}{\text{mass of exchanger}}$$

$D_g$  remains constant over a wide range of resin to liquid ratios. In a relatively short time, by simple equilibration of small known amounts of resin and solution followed by analysis of the phases, the distribution of solutes may be followed under many different sets of experimental conditions. Variables requiring investigation include the capacity and percent cross-linkage of resin, the type of resin itself, the temperature, and the concentration and pH of electrolyte in the equilibrating solution.

By comparing the ratio of the distribution coefficients for a pair of ions, a separation factor (or relative retention) is obtained for a specific experimental condition.

Instead of using  $D_g$ , separation data may be expressed in terms of a volume distribution coefficient  $D_v$ , which is defined as the amount of solution in the exchanger per cubic centimeter of resin bed divided by the amount per cubic centimeter in the liquid phase. The relation between  $D_g$  and  $D_v$  is given by:

$$D_v = D_g \rho$$

where  $\rho$  is the bed density of a column expressed in the units of mass of dry resin per cubic centimeter of column. The bed density can be determined by adding a known weight of dry resin to a graduated cylinder containing the eluting solution. After the resin has swelled to its maximum, a direct reading of the settled volume of resin is recorded.

Intelligent inspection of the relevant distribution coefficients will show whether a separation is feasible and what the most favorable eluant concentration is likely to be. In the columnar mode, an ion, even if not eluted, may move down the column a considerable distance and with the next eluant may appear in the eluate much earlier than indicated by the coefficient in the first eluant alone. A

distribution coefficient value of 12 or lower is required to elute an ion completely from a column containing about 10 g of dry resin using 250 to 300 mL of eluant. A larger volume of eluant is required only when exceptionally strong tailing occurs. Ions may be eluted completely by 300 to 400 mL of eluant from a column of 10 g of dry resin at  $D_g$  values of around 20. The first traces of an element will appear in the eluate at around 300 mL when its  $D_g$  value is about 50 to 60.

*Example* Shaking 50 mL of 0.001  $M$  cesium salt solution with 1.0 g of a strong cation exchanger in the H-form (with a capacity of 3.0 mequiv  $\cdot$  g $^{-1}$ ) removes the following amount of cesium. The selectivity coefficient,  $k_{Cs/H}$ , is 2.56, thus:

$$\frac{[Cs^+]_r[H^+]}{[Cs^+][H^+]_r} = 2.56$$

The maximum amount of cesium which can enter the resin is 50 mL  $\times$  0.001  $M$  = 0.050 equiv. The minimum value of  $[H^+]_r$  = 3.00 – 0.05 = 2.95 mequiv, and the maximum value, assuming complete exchange of cesium ion for hydrogen ion, is 0.001  $M$ . The minimum value of the distribution ratio is:

$$(D_c)_{Cs} = \frac{[Cs^+]_r}{[Cs^+]} = \frac{(2.56)(2.95)}{0.001} = 7550$$

$$\frac{\text{Amount of Cs, resin phase}}{\text{Amount of Cs, solution phase}} = \frac{(7550)(1.0 \text{ g})}{50 \text{ mL}} = 151$$

Thus, at equilibrium the 1.0 g of resin removed is:

$$\frac{100\% - x}{x} = 151$$

with all but 0.66% of cesium ions from solution. If the amount of resin were increased to 2.0 g, the amount of cesium remaining in solution would decrease to 0.33%, half the former value. However, if the depleted solution were decanted and placed in contact with 1 g of fresh resin, the amount of cesium remaining in solution would decrease to 0.004%. Two batch equilibrations would effectively remove the cesium from the solution.

11.5 GRAVIMETRIC ANALYSIS

TABLE 11.19 Gravimetric Factors

In the following table the elements are arranged in alphabetical order.  
Example: To convert a given weight of  $\text{Al}_2\text{O}_3$  to its equivalent of Al, multiply by the factor at the right, 0.52926; similarly to convert Al to  $\text{Al}_2\text{O}_3$ , multiply by the factor at the left, 1.8894.

| Factor                           |                                                                                                                                | Factor   |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------|----------|
| <b>ALUMINUM</b>                  |                                                                                                                                |          |
| <b>Al = 26.9815</b>              |                                                                                                                                |          |
| 0.74971                          | $\text{Al} \leftrightarrow \text{Al}_4\text{C}_3$                                                                              | 1.3341   |
| 0.058728                         | $\text{Al} \leftrightarrow \text{Al}(\text{C}_9\text{H}_6\text{ON})_3 \text{ (oxinate)}$                                       | 17.027   |
| 0.65829                          | $\text{Al} \leftrightarrow \text{AlN}$                                                                                         | 1.5191   |
| 1.8894                           | $\text{Al}_2\text{O}_3 \leftrightarrow \text{Al}$                                                                              | 0.52926  |
| 1.4165                           | $\text{Al}_2\text{O}_3 \leftrightarrow \text{Al}_4\text{C}_3$                                                                  | 0.70596  |
| 0.38233                          | $\text{Al}_2\text{O}_3 \leftrightarrow \text{AlCl}_3$                                                                          | 2.6155   |
| 0.41804                          | $\text{Al}_2\text{O}_3 \leftrightarrow \text{AlPO}_4$                                                                          | 2.3921   |
| 0.29800                          | $\text{Al}_2\text{O}_3 \leftrightarrow \text{Al}_2(\text{SO}_4)_3$                                                             | 3.3557   |
| 0.15300                          | $\text{Al}_2\text{O}_3 \leftrightarrow \text{Al}_2(\text{SO}_4)_3 \cdot 18\text{H}_2\text{O}$                                  | 6.5361   |
| 0.10746                          | $\text{Al}_2\text{O}_3 \leftrightarrow \text{K}_2\text{SO}_4 \cdot \text{Al}_2(\text{SO}_4)_3 \cdot 24\text{H}_2\text{O}$      | 9.3055   |
| 0.11246                          | $\text{Al}_2\text{O}_3 \leftrightarrow (\text{NH}_4)_2\text{SO}_4 \cdot \text{Al}_2(\text{SO}_4)_3 \cdot 24\text{H}_2\text{O}$ | 8.8922   |
| 4.5197                           | $\text{AlPO}_4 \leftrightarrow \text{Al}$                                                                                      | 0.22125  |
| 1.3946                           | $\text{CaF}_2 \leftrightarrow \text{AlF}_3$                                                                                    | 0.71704  |
| 0.58196                          | $\text{P}_2\text{O}_5 \leftrightarrow \text{AlPO}_4$                                                                           | 1.7183   |
| <b>AMMONIUM</b>                  |                                                                                                                                |          |
| <b>NH<sub>4</sub> = 18.03858</b> |                                                                                                                                |          |
| 1.1013                           | $\text{Ag} \leftrightarrow \text{NH}_4\text{Br}$                                                                               | 0.90802  |
| 2.0166                           | $\text{Ag} \leftrightarrow \text{NH}_4\text{Cl}$                                                                               | 0.49590  |
| 0.74424                          | $\text{Ag} \leftrightarrow \text{NH}_4\text{I}$                                                                                | 1.3437   |
| 1.9171                           | $\text{AgBr} \leftrightarrow \text{NH}_4\text{Br}$                                                                             | 0.52161  |
| 2.6792                           | $\text{AgCl} \leftrightarrow \text{NH}_4\text{Cl}$                                                                             | 0.37323  |
| 1.6198                           | $\text{AgI} \leftrightarrow \text{NH}_4\text{I}$                                                                               | 0.61737  |
| 1.7663                           | $\text{BaSO}_4 \leftrightarrow (\text{NH}_4)_2\text{SO}_4$                                                                     | 0.56615  |
| 0.81583                          | $\text{Br} \leftrightarrow \text{NH}_4\text{Br}$                                                                               | 1.2257   |
| 1.9654                           | $\text{Cl} \leftrightarrow \text{NH}_4$                                                                                        | 0.50881  |
| 0.66277                          | $\text{Cl} \leftrightarrow \text{NH}_4\text{Cl}$                                                                               | 1.5088   |
| 0.68162                          | $\text{HCl} \leftrightarrow \text{NH}_4\text{Cl}$                                                                              | 1.4671   |
| 0.87553                          | $\text{I} \leftrightarrow \text{NH}_4\text{I}$                                                                                 | 1.1422   |
| 14.410                           | $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O} \leftrightarrow \text{NH}_3$                                               | 0.069398 |
| 13.604                           | $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O} \leftrightarrow \text{NH}_4$                                               | 0.073506 |
| 9.4249                           | $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O} \leftrightarrow (\text{NH}_4)_2\text{O}$                                   | 0.10610  |
| 0.82244                          | $\text{N} \leftrightarrow \text{NH}_3$                                                                                         | 1.2159   |
| 0.77648                          | $\text{N} \leftrightarrow \text{NH}_4$                                                                                         | 1.2879   |
| 0.26185                          | $\text{N} \leftrightarrow \text{NH}_4\text{Cl}$                                                                                | 3.8189   |
| 0.17499                          | $\text{N} \leftrightarrow \text{NH}_4\text{NO}_3$                                                                              | 5.7145   |
| 0.53793                          | $\text{N} \leftrightarrow (\text{NH}_4)_2\text{O}$                                                                             | 1.8590   |
| 0.21200                          | $\text{N} \leftrightarrow (\text{NH}_4)_2\text{SO}_4$                                                                          | 4.7169   |
| 0.94412                          | $\text{NH}_3 \leftrightarrow \text{NH}_4$                                                                                      | 1.0592   |
| 0.35449                          | $\text{NH}_3 \leftrightarrow (\text{NH}_4)_2\text{CO}_3$                                                                       | 2.8210   |
| 0.21543                          | $\text{NH}_3 \leftrightarrow \text{NH}_4\text{HCO}_3$                                                                          | 4.6419   |
| 0.21277                          | $\text{NH}_3 \leftrightarrow \text{NH}_4\text{NO}_3$                                                                           | 4.6998   |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                           |                                                                                                          | Factor   |
|----------------------------------|----------------------------------------------------------------------------------------------------------|----------|
| <b>AMMONIUM (continued)</b>      |                                                                                                          |          |
| <b>NH<sub>4</sub> = 18.03858</b> |                                                                                                          |          |
| 0.65407                          | NH <sub>3</sub> ↔ (NH <sub>4</sub> ) <sub>2</sub> O                                                      | 1.5289   |
| 0.48596                          | NH <sub>3</sub> ↔ NH <sub>4</sub> OH                                                                     | 2.0578   |
| 0.25777                          | NH <sub>3</sub> ↔ (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>                                        | 3.8794   |
| 3.1409                           | NH <sub>4</sub> Cl ↔ NH <sub>3</sub>                                                                     | 0.31838  |
| 2.9654                           | NH <sub>4</sub> Cl ↔ NH <sub>4</sub>                                                                     | 0.33723  |
| 2.0543                           | NH <sub>4</sub> Cl ↔ (NH <sub>4</sub> ) <sub>2</sub> O                                                   | 0.48677  |
| 1.5263                           | NH <sub>4</sub> Cl ↔ NH <sub>4</sub> OH                                                                  | 0.65516  |
| 2.5020                           | NH <sub>4</sub> OH ↔ N                                                                                   | 0.39967  |
| 1.9428                           | NH <sub>4</sub> OH ↔ NH <sub>4</sub>                                                                     | 0.51472  |
| 13.032                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ NH <sub>3</sub>                                      | 0.076737 |
| 12.303                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ NH <sub>4</sub>                                      | 0.081279 |
| 4.1490                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ NH <sub>4</sub> Cl                                   | 0.24102  |
| 2.7728                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ NH <sub>4</sub> NO <sub>3</sub>                      | 0.36065  |
| 8.5235                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ (NH <sub>4</sub> ) <sub>2</sub> O                    | 0.11732  |
| 6.3328                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ NH <sub>4</sub> OH                                   | 0.15791  |
| 3.3592                           | (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> ↔ (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>      | 0.29769  |
| 1.3473                           | (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> ↔ H <sub>2</sub> SO <sub>4</sub>                         | 0.74223  |
| 3.1710                           | N <sub>2</sub> O <sub>5</sub> ↔ NH <sub>3</sub>                                                          | 0.31536  |
| 0.67470                          | N <sub>2</sub> O <sub>5</sub> ↔ NH <sub>4</sub> NO <sub>3</sub>                                          | 1.4821   |
| 2.0740                           | N <sub>2</sub> O <sub>5</sub> ↔ (NH <sub>4</sub> ) <sub>2</sub> O                                        | 0.48215  |
| 5.7275                           | Pt ↔ NH <sub>3</sub>                                                                                     | 0.17460  |
| 5.4074                           | Pt ↔ NH <sub>4</sub>                                                                                     | 0.18493  |
| 1.8235                           | Pt ↔ NH <sub>4</sub> Cl                                                                                  | 0.54838  |
| 1.2187                           | Pt ↔ NH <sub>4</sub> NO <sub>3</sub>                                                                     | 0.82058  |
| 3.7462                           | Pt ↔ (NH <sub>4</sub> ) <sub>2</sub> O                                                                   | 0.26694  |
| 2.7833                           | Pt ↔ NH <sub>4</sub> OH                                                                                  | 0.35928  |
| 1.4764                           | Pt ↔ (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>                                                     | 0.67733  |
| 2.3505                           | SO <sub>3</sub> ↔ NH <sub>3</sub>                                                                        | 0.42545  |
| 0.60589                          | SO <sub>3</sub> ↔ (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>                                        | 1.6505   |
| <b>ANTIMONY</b>                  |                                                                                                          |          |
| <b>Sb = 121.760</b>              |                                                                                                          |          |
| 0.36460                          | Sb ↔ KSbO · C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · ½H <sub>2</sub> O                             | 2.7428   |
| 0.83535                          | Sb ↔ Sb <sub>2</sub> O <sub>4</sub>                                                                      | 1.1971   |
| 0.75271                          | Sb ↔ Sb <sub>2</sub> O <sub>5</sub>                                                                      | 1.3285   |
| 0.43646                          | Sb <sub>2</sub> O <sub>3</sub> ↔ KSbO · C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · ½H <sub>2</sub> O | 2.2912   |
| 0.90106                          | Sb <sub>2</sub> O <sub>3</sub> ↔ Sb <sub>2</sub> O <sub>5</sub>                                          | 1.1098   |
| 0.72184                          | Sb <sub>2</sub> O <sub>3</sub> ↔ Sb <sub>2</sub> S <sub>5</sub>                                          | 1.3853   |
| 0.46042                          | Sb <sub>2</sub> O <sub>4</sub> ↔ KSbO · C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · ½H <sub>2</sub> O | 2.1719   |
| 1.2628                           | Sb <sub>2</sub> O <sub>4</sub> ↔ Sb                                                                      | 0.79188  |
| 1.0549                           | Sb <sub>2</sub> O <sub>4</sub> ↔ Sb <sub>2</sub> O <sub>3</sub>                                          | 0.94796  |
| 0.95053                          | Sb <sub>2</sub> O <sub>4</sub> ↔ Sb <sub>2</sub> O <sub>5</sub>                                          | 1.0520   |
| 0.90523                          | Sb <sub>2</sub> O <sub>4</sub> ↔ Sb <sub>2</sub> S <sub>3</sub>                                          | 1.1047   |
| 0.76147                          | Sb <sub>2</sub> O <sub>4</sub> ↔ Sb <sub>2</sub> S <sub>5</sub>                                          | 1.3133   |
| 0.80110                          | Sb <sub>2</sub> O <sub>5</sub> ↔ Sb <sub>2</sub> S <sub>5</sub>                                          | 1.2483   |
| 0.50862                          | Sb <sub>2</sub> S <sub>3</sub> ↔ KSbO · C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · ½H <sub>2</sub> O | 1.9661   |
| 1.3950                           | Sb <sub>2</sub> S <sub>3</sub> ↔ Sb                                                                      | 0.71683  |
| 1.1653                           | Sb <sub>2</sub> S <sub>3</sub> ↔ Sb <sub>2</sub> O <sub>3</sub>                                          | 0.85812  |
| 1.0500                           | Sb <sub>2</sub> S <sub>3</sub> ↔ Sb <sub>2</sub> O <sub>5</sub>                                          | 0.95234  |
| 1.6584                           | Sb <sub>2</sub> S <sub>5</sub> ↔ Sb                                                                      | 0.60299  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor              |                                                                                                       | Factor  |
|---------------------|-------------------------------------------------------------------------------------------------------|---------|
| <b>ARSENIC</b>      |                                                                                                       |         |
| <b>As = 74.9216</b> |                                                                                                       |         |
| 1.3203              | $\text{As}_2\text{O}_3 \leftrightarrow \text{As}$                                                     | 0.75738 |
| 0.86079             | $\text{As}_2\text{O}_3 \leftrightarrow \text{As}_2\text{O}_5$                                         | 1.1617  |
| 1.5339              | $\text{As}_2\text{O}_5 \leftrightarrow \text{As}$                                                     | 0.65195 |
| 1.6420              | $\text{As}_2\text{S}_3 \leftrightarrow \text{As}$                                                     | 0.60903 |
| 1.2436              | $\text{As}_2\text{S}_3 \leftrightarrow \text{As}_2\text{O}_3$                                         | 0.80413 |
| 1.0705              | $\text{As}_2\text{S}_3 \leftrightarrow \text{As}_2\text{O}_5$                                         | 0.93418 |
| 0.79324             | $\text{As}_2\text{S}_3 \leftrightarrow \text{As}_2\text{S}_5$                                         | 1.2606  |
| 2.0699              | $\text{As}_2\text{S}_5 \leftrightarrow \text{As}$                                                     | 0.48311 |
| 1.5678              | $\text{As}_2\text{S}_5 \leftrightarrow \text{As}_2\text{O}_3$                                         | 0.63787 |
| 1.3495              | $\text{As}_2\text{S}_5 \leftrightarrow \text{As}_2\text{O}_5$                                         | 0.74103 |
| 4.6729              | $\text{BaSO}_4 \leftrightarrow \text{As}$                                                             | 0.21400 |
| 3.5392              | $\text{BaSO}_4 \leftrightarrow \text{As}_2\text{O}_3$                                                 | 0.28255 |
| 3.0465              | $\text{BaSO}_4 \leftrightarrow \text{As}_2\text{O}_6$                                                 | 0.32825 |
| 2.8482              | $\text{BaSO}_4 \leftrightarrow \text{AsO}_3$                                                          | 0.35110 |
| 2.5202              | $\text{BaSO}_4 \leftrightarrow \text{AsO}_4$                                                          | 0.39680 |
| 2.0719              | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{As}$                                          | 0.48265 |
| 1.5692              | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{As}_2\text{O}_3$                              | 0.63726 |
| 1.3509              | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{As}_2\text{O}_5$                              | 0.74032 |
| 1.2629              | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{AsO}_2$                                       | 0.79186 |
| 1.1174              | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{AsO}_4$                                       | 0.89493 |
| 1.2619              | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{As}_2\text{S}_3$                              | 0.79249 |
| 2.5397              | $\text{MgNH}_4\text{AsO}_4 \cdot \frac{1}{2}\text{H}_2\text{O} \leftrightarrow \text{As}$             | 0.39374 |
| 1.9235              | $\text{MgNH}_4\text{AsO}_4 \cdot \frac{1}{2}\text{H}_2\text{O} \leftrightarrow \text{As}_2\text{O}_3$ | 0.51988 |
| 1.6558              | $\text{MgNH}_4\text{AsO}_4 \cdot \frac{1}{2}\text{H}_2\text{O} \leftrightarrow \text{As}_2\text{O}_5$ | 0.60395 |
| 1.5480              | $\text{MgNH}_4\text{AsO}_4 \cdot \frac{1}{2}\text{H}_2\text{O} \leftrightarrow \text{AsO}_3$          | 0.64600 |
| 1.3697              | $\text{MgNH}_4\text{AsO}_4 \cdot \frac{1}{2}\text{H}_2\text{O} \leftrightarrow \text{AsO}_4$          | 0.73008 |
| <b>BARIUM</b>       |                                                                                                       |         |
| <b>Ba = 137.34</b>  |                                                                                                       |         |
| 1.4369              | $\text{BaCO}_3 \leftrightarrow \text{Ba}$                                                             | 0.69592 |
| 0.94766             | $\text{BaCO}_3 \leftrightarrow \text{BaCl}_2$                                                         | 1.0552  |
| 0.76088             | $\text{BaCO}_3 \leftrightarrow \text{Ba}(\text{HCO}_3)_2$                                             | 1.3143  |
| 1.2871              | $\text{BaCO}_3 \leftrightarrow \text{BaO}$                                                            | 0.77699 |
| 1.8446              | $\text{BaCrO}_4 \leftrightarrow \text{Ba}$                                                            | 0.54214 |
| 1.2165              | $\text{BaCrO}_4 \leftrightarrow \text{BaCl}_2$                                                        | 0.82205 |
| 1.2838              | $\text{BaCrO}_4 \leftrightarrow \text{BaCO}_3$                                                        | 0.77902 |
| 1.6521              | $\text{BaCrO}_4 \leftrightarrow \text{BaO}$                                                           | 0.60530 |
| 2.0345              | $\text{BaSiF}_6 \leftrightarrow \text{Ba}$                                                            | 0.49152 |
| 1.5936              | $\text{BaSiF}_6 \leftrightarrow \text{BaF}_2$                                                         | 0.62751 |
| 1.8222              | $\text{BaSiF}_6 \leftrightarrow \text{BaO}$                                                           | 0.54878 |
| 1.6994              | $\text{BaSO}_4 \leftrightarrow \text{Ba}$                                                             | 0.58843 |
| 1.1208              | $\text{BaSO}_4 \leftrightarrow \text{BaCl}_2$                                                         | 0.89224 |
| 0.95546             | $\text{BaSO}_4 \leftrightarrow \text{BaCl}_2 \cdot 2\text{H}_2\text{O}$                               | 1.0466  |
| 1.1827              | $\text{BaSO}_4 \leftrightarrow \text{BaCO}_3$                                                         | 0.84554 |
| 0.89308             | $\text{BaSO}_4 \leftrightarrow \text{Ba}(\text{NO}_3)_2$                                              | 1.1197  |
| 1.5221              | $\text{BaSO}_4 \leftrightarrow \text{BaO}$                                                            | 0.65698 |
| 1.3783              | $\text{BaSO}_4 \leftrightarrow \text{BaO}_2$                                                          | 0.72554 |
| 1.3778              | $\text{BaSO}_4 \leftrightarrow \text{BaS}$                                                            | 0.72579 |
| 0.28701             | $\text{CO}_2 \leftrightarrow \text{BaO}$                                                              | 3.4842  |
| 0.22300             | $\text{CO}_2 \leftrightarrow \text{BaCO}_3$                                                           | 4.4842  |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor              |                                                                                                   | Factor   |
|---------------------|---------------------------------------------------------------------------------------------------|----------|
| <b>BERYLLIUM</b>    |                                                                                                   |          |
| <b>Be = 9.0122</b>  |                                                                                                   |          |
| 8.8678              | $\text{BeCl}_2 \leftrightarrow \text{Be}$                                                         | 0.11277  |
| 2.7753              | $\text{BeO} \leftrightarrow \text{Be}$                                                            | 0.36033  |
| 0.31296             | $\text{BeO} \leftrightarrow \text{BeCl}_2$                                                        | 3.1953   |
| 0.14119             | $\text{BeO} \leftrightarrow \text{BeSO}_4 \cdot 4\text{H}_2\text{O}$                              | 7.0825   |
| <b>BISMUTH</b>      |                                                                                                   |          |
| <b>Bi = 208.980</b> |                                                                                                   |          |
| 0.89699             | $\text{Bi} \leftrightarrow \text{Bi}_2\text{O}_3$                                                 | 1.1148   |
| 1.6648              | $\text{BiAsO}_4 \leftrightarrow \text{Bi}$                                                        | 0.60069  |
| 1.4933              | $\text{BiAsO}_4 \leftrightarrow \text{Bi}_2\text{O}_4$                                            | 0.66968  |
| 0.48030             | $\text{Bi}_2\text{O}_3 \leftrightarrow \text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$        | 2.0820   |
| 0.81183             | $\text{Bi}_2\text{O}_3 \leftrightarrow \text{BiONO}_3$                                            | 1.2318   |
| 1.2462              | $\text{BiOCl} \leftrightarrow \text{Bi}$                                                          | 0.80244  |
| 0.53689             | $\text{BiOCl} \leftrightarrow \text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$                 | 1.8626   |
| 1.1178              | $\text{BiOCl} \leftrightarrow \text{Bi}_2\text{O}_3$                                              | 0.89460  |
| 0.90748             | $\text{BiOCl} \leftrightarrow \text{BiONO}_3$                                                     | 1.1019   |
| 1.2301              | $\text{Bi}_2\text{S}_3 \leftrightarrow \text{Bi}$                                                 | 0.81291  |
| 1.1034              | $\text{Bi}_2\text{S}_3 \leftrightarrow \text{Bi}_2\text{O}_3$                                     | 0.90627  |
| <b>BORON</b>        |                                                                                                   |          |
| <b>B = 10.81</b>    |                                                                                                   |          |
| 3.2199              | $\text{B}_2\text{O}_3 \leftrightarrow \text{B}$                                                   | 0.31057  |
| 0.81317             | $\text{B}_2\text{O}_3 \leftrightarrow \text{BO}_2$                                                | 1.2298   |
| 0.59193             | $\text{B}_2\text{O}_3 \leftrightarrow \text{BO}_3$                                                | 1.6894   |
| 0.89693             | $\text{B}_2\text{O}_3 \leftrightarrow \text{B}_4\text{O}_7$                                       | 1.1149   |
| 0.56298             | $\text{B}_2\text{O}_3 \leftrightarrow \text{H}_3\text{BO}_3$                                      | 1.7763   |
| 0.36510             | $\text{B}_2\text{O}_3 \leftrightarrow \text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$ | 2.7389   |
| 6.4005              | $\text{B}_6\text{C} \leftrightarrow \text{C}$                                                     | 0.15624  |
| 11.646              | $\text{KBF}_4 \leftrightarrow \text{B}$                                                           | 0.085863 |
| 3.6171              | $\text{KBF}_4 \leftrightarrow \text{B}_2\text{O}_3$                                               | 0.27647  |
| 2.0363              | $\text{KBF}_4 \leftrightarrow \text{H}_3\text{BO}_3$                                              | 0.49108  |
| 1.3206              | $\text{KBF}_4 \leftrightarrow \text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$         | 0.75723  |
| <b>BROMINE</b>      |                                                                                                   |          |
| <b>Br = 79.90</b>   |                                                                                                   |          |
| 1.3499              | $\text{Ag} \leftrightarrow \text{Br}$                                                             | 0.74079  |
| 0.84333             | $\text{Ag} \leftrightarrow \text{BrO}_3$                                                          | 1.1858   |
| 1.3331              | $\text{Ag} \leftrightarrow \text{HBr}$                                                            | 0.75013  |
| 2.3499              | $\text{AgBr} \leftrightarrow \text{Br}$                                                           | 0.42555  |
| 1.4681              | $\text{AgBr} \leftrightarrow \text{BrO}_3$                                                        | 0.68117  |
| 2.3206              | $\text{AgBr} \leftrightarrow \text{HBr}$                                                          | 0.43091  |
| 0.55756             | $\text{Br} \leftrightarrow \text{AgCl}$                                                           | 1.7935   |
| 9.9892              | $\text{Br} \leftrightarrow \text{O}$                                                              | 0.10010  |
| 1.1858              | $\text{BrO}_3 \leftrightarrow \text{Ag}$                                                          | 0.84333  |
| <b>CADMIUM</b>      |                                                                                                   |          |
| <b>Cd = 112.40</b>  |                                                                                                   |          |
| 0.61317             | $\text{Cd} \leftrightarrow \text{CdCl}_2$                                                         | 1.6309   |
| 0.47545             | $\text{Cd} \leftrightarrow \text{Cd}(\text{NO}_3)_2$                                              | 2.1033   |
| 1.1423              | $\text{CdO} \leftrightarrow \text{Cd}$                                                            | 0.87539  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                              |                                                                                              | Factor   |
|-------------------------------------|----------------------------------------------------------------------------------------------|----------|
| <b>CADMIUM</b> ( <i>continued</i> ) |                                                                                              |          |
| <b>Cd = 112.40</b>                  |                                                                                              |          |
| 0.70045                             | $\text{CdO} \leftrightarrow \text{CdCl}_2$                                                   | 1.4276   |
| 0.54312                             | $\text{CdO} \leftrightarrow \text{Cd}(\text{NO}_3)_2$                                        | 1.8412   |
| 1.2852                              | $\text{CdS} \leftrightarrow \text{Cd}$                                                       | 0.77807  |
| 0.78806                             | $\text{CdS} \leftrightarrow \text{CdCl}_2$                                                   | 1.2689   |
| 0.61106                             | $\text{CdS} \leftrightarrow \text{Cd}(\text{NO}_3)_2$                                        | 1.6365   |
| 1.1251                              | $\text{CdS} \leftrightarrow \text{CdO}$                                                      | 0.88883  |
| 0.69298                             | $\text{CdS} \leftrightarrow \text{CdSO}_4$                                                   | 1.4430   |
| 1.8546                              | $\text{CdSO}_4 \leftrightarrow \text{Cd}$                                                    | 0.53919  |
| 1.1372                              | $\text{CdSO}_4 \leftrightarrow \text{CdCl}_2$                                                | 0.87935  |
| 0.88177                             | $\text{CdSO}_4 \leftrightarrow \text{Cd}(\text{NO}_3)_2$                                     | 1.1341   |
| 1.6235                              | $\text{CdSO}_4 \leftrightarrow \text{CdO}$                                                   | 0.61595  |
| <b>CALCIUM</b>                      |                                                                                              |          |
| <b>Ca = 40.08</b>                   |                                                                                              |          |
| 3.2352                              | $\text{BaSO}_4 \leftrightarrow \text{CaS}$                                                   | 0.30910  |
| 1.7144                              | $\text{BaSO}_4 \leftrightarrow \text{CaSO}_4$                                                | 0.58329  |
| 1.3556                              | $\text{BaSO}_4 \leftrightarrow \text{CaSO}_4 \cdot 2\text{H}_2\text{O}$                      | 0.73766  |
| 0.36111                             | $\text{Ca} \leftrightarrow \text{CaCl}_2$                                                    | 2.7692   |
| 0.51334                             | $\text{Ca} \leftrightarrow \text{CaF}_2$                                                     | 1.9480   |
| 0.71471                             | $\text{Ca} \leftrightarrow \text{CaO}$                                                       | 1.3992   |
| 2.4973                              | $\text{CaCO}_3 \leftrightarrow \text{Ca}$                                                    | 0.40044  |
| 0.90179                             | $\text{CaCO}_3 \leftrightarrow \text{CaCl}_2$                                                | 1.1089   |
| 0.61742                             | $\text{CaCO}_3 \leftrightarrow \text{Ca}(\text{HCO}_3)_2$                                    | 1.6196   |
| 1.7848                              | $\text{CaCO}_3 \leftrightarrow \text{CaO}$                                                   | 0.56029  |
| 0.73520                             | $\text{CaCO}_3 \leftrightarrow \text{CaSO}_4$                                                | 1.3602   |
| 0.58134                             | $\text{CaCO}_3 \leftrightarrow \text{CaSO}_4 \cdot 2\text{H}_2\text{O}$                      | 1.7202   |
| 1.3726                              | $\text{CaCO}_3 \leftrightarrow \text{HCl}$                                                   | 0.72856  |
| 0.50526                             | $\text{CaO} \leftrightarrow \text{CaCl}_2$                                                   | 1.9792   |
| 0.71825                             | $\text{CaO} \leftrightarrow \text{CaF}_2$                                                    | 1.3923   |
| 0.34593                             | $\text{CaO} \leftrightarrow \text{Ca}(\text{HCO}_3)_2$                                       | 2.8907   |
| 0.75685                             | $\text{CaO} \leftrightarrow \text{Ca}(\text{OH})_2$                                          | 1.3213   |
| 0.41192                             | $\text{CaO} \leftrightarrow \text{CaSO}_4$                                                   | 2.4276   |
| 0.32572                             | $\text{CaO} \leftrightarrow \text{CaSO}_4 \cdot 2\text{H}_2\text{O}$                         | 3.0701   |
| 2.5797                              | $\text{Ca}_3(\text{PO}_4)_2 \leftrightarrow \text{Ca}$                                       | 0.38765  |
| 1.8437                              | $\text{Ca}_3(\text{PO}_4)_2 \leftrightarrow \text{CaO}$                                      | 0.54239  |
| 0.75946                             | $\text{Ca}_3(\text{PO}_4)_2 \leftrightarrow \text{CaSO}_4$                                   | 1.3167   |
| 3.3967                              | $\text{CaSO}_4 \leftrightarrow \text{Ca}$                                                    | 0.29440  |
| 1.2266                              | $\text{CaSO}_4 \leftrightarrow \text{CaCl}_2$                                                | 0.81526  |
| 1.3602                              | $\text{CaSO}_4 \leftrightarrow \text{CaCO}_3$                                                | 0.73520  |
| 1.7437                              | $\text{CaSO}_4 \leftrightarrow \text{CaF}_2$                                                 | 0.57351  |
| 2.4276                              | $\text{CaSO}_4 \leftrightarrow \text{CaO}$                                                   | 0.41192  |
| 1.7691                              | $\text{Cl} \leftrightarrow \text{Ca}$                                                        | 0.56526  |
| 0.63885                             | $\text{Cl} \leftrightarrow \text{CaCl}_2$                                                    | 1.5653   |
| 1.2644                              | $\text{Cl} \leftrightarrow \text{CaO}$                                                       | 0.79089  |
| 0.78479                             | $\text{CO}_2 \leftrightarrow \text{CaO}$                                                     | 1.2742   |
| 0.43970                             | $\text{CO}_2 \leftrightarrow \text{CaCO}_3$                                                  | 2.2743   |
| 0.77989                             | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{Ca}_3(\text{AsO}_4)_2$               | 1.2822   |
| 0.71883                             | $\text{MgO} \leftrightarrow \text{CaO}$                                                      | 1.3912   |
| 0.71755                             | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Ca}_3(\text{PO}_4)_2$                 | 1.3936   |
| 12.098                              | $(\text{NH}_4)_3\text{PO}_4 \cdot 12\text{MoO}_3 \leftrightarrow \text{Ca}_3(\text{PO}_4)_2$ | 0.082657 |



TABLE 11.19 Gravimetric Factors (Continued)

| Factor              |                                                                       | Factor   |
|---------------------|-----------------------------------------------------------------------|----------|
| CALCIUM (continued) |                                                                       |          |
| Ca = 40.08          |                                                                       |          |
| 0.65824             | $\text{N}_2\text{O}_5 \leftrightarrow \text{Ca}(\text{NO}_3)_2$       | 1.5192   |
| 0.45761             | $\text{P}_2\text{O}_3 \leftrightarrow \text{Ca}_3(\text{PO}_4)_2$     | 2.1853   |
| 1.4277              | $\text{SO}_3 \leftrightarrow \text{CaO}$                              | 0.70044  |
| 0.58809             | $\text{SO}_3 \leftrightarrow \text{CaSO}_4$                           | 1.7004   |
| 0.46502             | $\text{SO}_3 \leftrightarrow \text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ | 2.1505   |
| 0.80523             | $\text{WO}_3 \leftrightarrow \text{CaWO}_4$                           | 1.2419   |
| CARBON              |                                                                       |          |
| C = 12.011          |                                                                       |          |
| 3.9913              | $\text{Ag} \leftrightarrow \text{HCN}$                                | 0.25054  |
| 1.6565              | $\text{Ag} \leftrightarrow \text{KCN}$                                | 0.60369  |
| 4.9541              | $\text{AgCN} \leftrightarrow \text{HCN}$                              | 0.20185  |
| 2.0561              | $\text{AgCN} \leftrightarrow \text{KCN}$                              | 0.48637  |
| 16.431              | $\text{BaCO}_3 \leftrightarrow \text{C}$                              | 0.060861 |
| 4.4842              | $\text{BaCO}_3 \leftrightarrow \text{CO}_2$                           | 0.22301  |
| 3.2887              | $\text{BaCO}_3 \leftrightarrow \text{CO}_3$                           | 0.30407  |
| 3.4842              | $\text{BaO} \leftrightarrow \text{CO}_2$                              | 0.28701  |
| 1.7421              | $\text{BaO} \leftrightarrow \text{CO}_2, \text{ bicarbonate}$         | 0.57402  |
| 0.19432             | $\text{CN} \leftrightarrow \text{AgCN}$                               | 5.1461   |
| 0.24120             | $\text{CN} \leftrightarrow \text{Ag}$                                 | 4.1460   |
| 0.35000             | $\text{SCN} \leftrightarrow \text{AgSCN}$                             | 2.8572   |
| 0.47757             | $\text{SCN} \leftrightarrow \text{CuSCN}$                             | 2.0939   |
| 0.24885             | $\text{SCN} \leftrightarrow \text{BaSO}_4$                            | 4.0185   |
| 1.2742              | $\text{CaO} \leftrightarrow \text{CO}_2$                              | 0.78479  |
| 0.63712             | $\text{CaO} \leftrightarrow \text{CO}_2, \text{ bicarbonate}$         | 1.5696   |
| 0.33936             | $\text{CO}_2 \leftrightarrow \text{Ba}(\text{HCO}_3)_2$               | 2.9467   |
| 3.6641              | $\text{CO}_2 \leftrightarrow \text{C}$                                | 0.27291  |
| 0.43970             | $\text{CO}_2 \leftrightarrow \text{CaCO}_3$                           | 2.2743   |
| 0.54297             | $\text{CO}_2 \leftrightarrow \text{Ca}(\text{HCO}_3)_2$               | 1.8417   |
| 0.73341             | $\text{CO}_2 \leftrightarrow \text{CO}_3$                             | 1.3635   |
| 0.13507             | $\text{CO}_2 \leftrightarrow \text{Cs}_2\text{CO}_3$                  | 7.4033   |
| 0.22695             | $\text{CO}_2 \leftrightarrow \text{CsHCO}_3$                          | 4.4063   |
| 0.37986             | $\text{CO}_2 \leftrightarrow \text{FeCO}_3$                           | 2.6326   |
| 0.49483             | $\text{CO}_2 \leftrightarrow \text{Fe}(\text{HCO}_3)_2$               | 2.0209   |
| 0.31843             | $\text{CO}_2 \leftrightarrow \text{K}_2\text{CO}_3$                   | 3.1404   |
| 0.43957             | $\text{CO}_2 \leftrightarrow \text{KHCO}_3$                           | 2.2749   |
| 0.46718             | $\text{CO}_2 \leftrightarrow \text{K}_2\text{O}$                      | 2.1405   |
| 0.59564             | $\text{CO}_2 \leftrightarrow \text{Li}_2\text{CO}_3$                  | 1.6789   |
| 0.64762             | $\text{CO}_2 \leftrightarrow \text{LiHCO}_3$                          | 1.5441   |
| 1.4730              | $\text{CO}_2 \leftrightarrow \text{Li}_2\text{O}$                     | 0.67887  |
| 0.52193             | $\text{CO}_2 \leftrightarrow \text{MgCO}_3$                           | 1.9159   |
| 0.60143             | $\text{CO}_2 \leftrightarrow \text{Mg}(\text{HCO}_3)_2$               | 1.6627   |
| 1.0918              | $\text{CO}_2 \leftrightarrow \text{MgO}$                              | 0.91595  |
| 0.38286             | $\text{CO}_2 \leftrightarrow \text{MnCO}_3$                           | 2.6119   |
| 0.49737             | $\text{CO}_2 \leftrightarrow \text{Mn}(\text{HCO}_3)_2$               | 2.0106   |
| 0.62041             | $\text{CO}_2 \leftrightarrow \text{MnO}$                              | 1.6118   |
| 0.41523             | $\text{CO}_2 \leftrightarrow \text{Na}_2\text{CO}_3$                  | 2.4083   |
| 0.52388             | $\text{CO}_2 \leftrightarrow \text{NaHCO}_3$                          | 1.9088   |
| 0.71008             | $\text{CO}_2 \leftrightarrow \text{Na}_2\text{O}$                     | 1.4083   |
| 0.45802             | $\text{CO}_2 \leftrightarrow (\text{NH}_4)_2\text{CO}_3$              | 2.1833   |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                             |                                                                                                                         | Factor  |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------|---------|
| <b>CARBON</b> ( <i>continued</i> ) |                                                                                                                         |         |
| <b>C = 12.011</b>                  |                                                                                                                         |         |
| 0.55669                            | $\text{CO}_2 \leftrightarrow \text{NH}_4\text{HCO}_3$                                                                   | 1.7963  |
| 0.16471                            | $\text{CO}_2 \leftrightarrow \text{PbCO}_3$                                                                             | 6.0713  |
| 0.19055                            | $\text{CO}_2 \leftrightarrow \text{Rb}_2\text{CO}_3$                                                                    | 5.2477  |
| 0.30043                            | $\text{CO}_2 \leftrightarrow \text{RbHCO}_3$                                                                            | 3.3286  |
| 0.23542                            | $\text{CO}_2 \leftrightarrow \text{Rb}_2\text{O}$                                                                       | 4.2477  |
| 0.29811                            | $\text{CO}_2 \leftrightarrow \text{SrCO}_3$                                                                             | 3.3545  |
| 0.41984                            | $\text{CO}_2 \leftrightarrow \text{Sr}(\text{HCO}_3)_2$                                                                 | 2.3818  |
| 0.42474                            | $\text{CO}_2 \leftrightarrow \text{SrO}$                                                                                | 2.3545  |
| <b>CERIUM</b>                      |                                                                                                                         |         |
| <b>Ce = 140.12</b>                 |                                                                                                                         |         |
| 0.36100                            | $\text{Ce} \leftrightarrow \text{Ce}(\text{NO}_3)_4$                                                                    | 2.7701  |
| 0.24746                            | $\text{Ce} \leftrightarrow \text{Ce}(\text{NO}_3)_4 \cdot 2\text{NH}_4\text{NO}_3 \cdot \text{H}_2\text{O}$             | 4.0411  |
| 0.81408                            | $\text{Ce} \leftrightarrow \text{CeO}_2$                                                                                | 1.2284  |
| 0.85377                            | $\text{Ce} \leftrightarrow \text{Ce}_2\text{O}_3$                                                                       | 1.1713  |
| 0.49302                            | $\text{Ce} \leftrightarrow \text{Ce}_2(\text{SO}_4)_3$                                                                  | 2.0283  |
| 1.0527                             | $\text{Ce}_2(\text{C}_2\text{O}_4)_3 \cdot 3\text{H}_2\text{O} \leftrightarrow \text{Ce}_2(\text{SO}_4)_3$              | 0.94998 |
| 2.1351                             | $\text{Ce}_2(\text{C}_2\text{O}_4)_3 \cdot 3\text{H}_2\text{O} \leftrightarrow \text{Ce}$                               | 0.46835 |
| 0.44345                            | $\text{CeO}_2 \leftrightarrow \text{Ce}(\text{NO}_3)_4$                                                                 | 2.2551  |
| 0.30397                            | $\text{CeO}_2 \leftrightarrow \text{Ce}(\text{NO}_3)_4 \cdot 2\text{NH}_4\text{NO}_3 \cdot \text{H}_2\text{O}$          | 3.2898  |
| 0.42284                            | $\text{Ce}_2\text{O}_3 \leftrightarrow \text{Ce}(\text{NO}_3)_4$                                                        | 2.3650  |
| 0.28984                            | $\text{Ce}_2\text{O}_3 \leftrightarrow \text{Ce}(\text{NO}_3)_4 \cdot 2\text{NH}_4\text{NO}_3 \cdot \text{H}_2\text{O}$ | 3.4502  |
| 0.95352                            | $\text{Ce}_2\text{O}_3 \leftrightarrow \text{CeO}_2$                                                                    | 1.0487  |
| 0.57746                            | $\text{Ce}_2\text{O}_3 \leftrightarrow \text{Ce}_2(\text{SO}_4)_3$                                                      | 1.7317  |
| <b>CESIUM</b>                      |                                                                                                                         |         |
| <b>Cs = 137.905</b>                |                                                                                                                         |         |
| 0.85127                            | $\text{AgCl} \leftrightarrow \text{CsCl}$                                                                               | 1.1747  |
| 0.26675                            | $\text{Cl} \leftrightarrow \text{Cs}$                                                                                   | 3.7489  |
| 0.21058                            | $\text{Cl} \leftrightarrow \text{CsCl}$                                                                                 | 4.7488  |
| 0.78944                            | $\text{Cs} \leftrightarrow \text{CsCl}$                                                                                 | 1.2667  |
| 0.57200                            | $\text{Cs} \leftrightarrow \text{CsClO}_4$                                                                              | 1.7483  |
| 0.81585                            | $\text{Cs} \leftrightarrow \text{Cs}_2\text{CO}_3$                                                                      | 1.2257  |
| 0.94326                            | $\text{Cs} \leftrightarrow \text{Cs}_2\text{O}$                                                                         | 1.0602  |
| 0.83693                            | $\text{Cs}_2\text{O} \leftrightarrow \text{CsCl}$                                                                       | 1.1948  |
| 0.77876                            | $\text{Cs}_2\text{O} \leftrightarrow \text{Cs}_2\text{SO}_4$                                                            | 1.2841  |
| 2.5341                             | $\text{Cs}_2\text{PtCl}_6 \leftrightarrow \text{Cs}$                                                                    | 0.39461 |
| 2.0005                             | $\text{Cs}_2\text{PtCl}_6 \leftrightarrow \text{CsCl}$                                                                  | 0.49987 |
| 2.0675                             | $\text{Cs}_2\text{PtCl}_6 \leftrightarrow \text{Cs}_2\text{CO}_3$                                                       | 0.48369 |
| 2.3903                             | $\text{Cs}_2\text{PtCl}_6 \leftrightarrow \text{Cs}_2\text{O}$                                                          | 0.41835 |
| 1.3613                             | $\text{Cs}_2\text{SO}_4 \leftrightarrow \text{Cs}$                                                                      | 0.73457 |
| 1.0747                             | $\text{Cs}_2\text{SO}_4 \leftrightarrow \text{CsCl}$                                                                    | 0.93050 |
| 1.1106                             | $\text{Cs}_2\text{SO}_4 \leftrightarrow \text{Cs}_2\text{CO}_3$                                                         | 0.90038 |
| 0.28410                            | $\text{SO}_3 \leftrightarrow \text{Cs}_2\text{O}$                                                                       | 3.5199  |
| <b>CHLORINE</b>                    |                                                                                                                         |         |
| <b>Cl = 35.453</b>                 |                                                                                                                         |         |
| 3.0426                             | $\text{Ag} \leftrightarrow \text{Cl}$                                                                                   | 0.32866 |
| 2.9585                             | $\text{Ag} \leftrightarrow \text{HCl}$                                                                                  | 0.33801 |
| 4.0425                             | $\text{AgCl} \leftrightarrow \text{Cl}$                                                                                 | 0.24737 |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                      |                                                                                        | Factor  |
|-----------------------------|----------------------------------------------------------------------------------------|---------|
| <b>CHLORINE (continued)</b> |                                                                                        |         |
| <b>Cl = 35.453</b>          |                                                                                        |         |
| 3.9308                      | $\text{AgCl} \leftrightarrow \text{HCl}$                                               | 0.25440 |
| 3.5728                      | $\text{BaCrO}_4 \leftrightarrow \text{Cl}$                                             | 0.27990 |
| 0.56526                     | $\text{Ca} \leftrightarrow \text{Cl}$                                                  | 1.7691  |
| 0.97235                     | $\text{Cl} \leftrightarrow \text{HCl}$                                                 | 1.0284  |
| 0.58227                     | $\text{ClO}_3 \leftrightarrow \text{AgCl}$                                             | 1.7174  |
| 1.1193                      | $\text{ClO}_3 \leftrightarrow \text{KCl}$                                              | 0.89340 |
| 1.4279                      | $\text{ClO}_3 \leftrightarrow \text{NaCl}$                                             | 0.70033 |
| 0.69391                     | $\text{ClO}_4 \leftrightarrow \text{AgCl}$                                             | 1.4411  |
| 1.3339                      | $\text{ClO}_4 \leftrightarrow \text{KCl}$                                              | 0.74967 |
| 1.7017                      | $\text{ClO}_4 \leftrightarrow \text{NaCl}$                                             | 0.58766 |
| 1.1029                      | $\text{K} \leftrightarrow \text{Cl}$                                                   | 0.90668 |
| 2.1029                      | $\text{KCl} \leftrightarrow \text{Cl}$                                                 | 0.47553 |
| 0.19572                     | $\text{Li} \leftrightarrow \text{Cl}$                                                  | 5.1092  |
| 0.34288                     | $\text{Mg} \leftrightarrow \text{Cl}$                                                  | 2.9165  |
| 1.3429                      | $\text{MgCl}_2 \leftrightarrow \text{Cl}$                                              | 0.74467 |
| 1.2261                      | $\text{MnO}_2 \leftrightarrow \text{Cl}$                                               | 0.81560 |
| 0.64846                     | $\text{Na} \leftrightarrow \text{Cl}$                                                  | 1.5421  |
| 1.6485                      | $\text{NaCl} \leftrightarrow \text{Cl}$                                                | 0.60663 |
| 0.50881                     | $\text{NH}_4 \leftrightarrow \text{Cl}$                                                | 1.9654  |
| 1.4671                      | $\text{NH}_4\text{Cl} \leftrightarrow \text{HCl}$                                      | 0.68162 |
| 1.8121                      | $(\text{NH}_4)_2\text{SO}_4 \leftrightarrow \text{HCl}$                                | 0.55185 |
| 4.5580                      | $\text{PbCrO}_4 \leftrightarrow \text{Cl}$                                             | 0.21939 |
| <b>CHROMIUM</b>             |                                                                                        |         |
| <b>Cr = 51.996</b>          |                                                                                        |         |
| 4.8721                      | $\text{BaCrO}_4 \leftrightarrow \text{Cr}$                                             | 0.20525 |
| 3.3335                      | $\text{BaCrO}_4 \leftrightarrow \text{Cr}_2\text{O}_3$                                 | 0.29998 |
| 2.5335                      | $\text{BaCrO}_4 \leftrightarrow \text{CrO}_3$                                          | 0.39472 |
| 2.1841                      | $\text{BaCrO}_4 \leftrightarrow \text{CrO}_4$                                          | 0.45786 |
| 0.70718                     | $\text{BaCrO}_4 \leftrightarrow \text{Cr}_2(\text{SO}_4)_3 \cdot 18\text{H}_2\text{O}$ | 1.4141  |
| 7.4935                      | $\text{Cr}_3\text{C}_2 \leftrightarrow \text{C}$                                       | 0.13345 |
| 1.9231                      | $\text{CrO}_3 \leftrightarrow \text{Cr}$                                               | 0.51999 |
| 1.4616                      | $\text{Cr}_2\text{O}_3 \leftrightarrow \text{Cr}$                                      | 0.68420 |
| 0.76000                     | $\text{Cr}_2\text{O}_3 \leftrightarrow \text{CrO}_3$                                   | 1.3158  |
| 0.65519                     | $\text{Cr}_2\text{O}_3 \leftrightarrow \text{CrO}_4$                                   | 1.5263  |
| 3.7349                      | $\text{K}_2\text{CrO}_4 \leftrightarrow \text{Cr}$                                     | 0.26774 |
| 1.9421                      | $\text{K}_2\text{CrO}_4 \leftrightarrow \text{CrO}_3$                                  | 0.51490 |
| 1.4710                      | $\text{K}_2\text{Cr}_2\text{O}_7 \leftrightarrow \text{CrO}_3$                         | 0.67979 |
| 6.2155                      | $\text{PbCrO}_4 \leftrightarrow \text{Cr}$                                             | 0.16089 |
| 4.2527                      | $\text{PbCrO}_4 \leftrightarrow \text{Cr}_2\text{O}_3$                                 | 0.23515 |
| 3.2320                      | $\text{PbCrO}_4 \leftrightarrow \text{CrO}_3$                                          | 0.30941 |
| 2.7863                      | $\text{PbCrO}_4 \leftrightarrow \text{CrO}_4$                                          | 0.35890 |
| 0.90217                     | $\text{PbCrO}_4 \leftrightarrow \text{Cr}_2(\text{SO}_4)_3 \cdot 18\text{H}_2\text{O}$ | 1.1084  |
| 1.6642                      | $\text{PbCrO}_4 \leftrightarrow \text{K}_2\text{CrO}_4$                                | 0.60090 |
| 2.1971                      | $\text{PbCrO}_4 \leftrightarrow \text{K}_2\text{Cr}_2\text{O}_7$                       | 0.45515 |
| <b>COBALT</b>               |                                                                                        |         |
| <b>Co = 58.9332</b>         |                                                                                        |         |
| 0.20249                     | $\text{Co} \leftrightarrow \text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$         | 4.9385  |
| 0.78648                     | $\text{Co} \leftrightarrow \text{CoO}$                                                 | 1.2715  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                             |                                                                                                              | Factor  |
|------------------------------------|--------------------------------------------------------------------------------------------------------------|---------|
| <b>COBALT</b> ( <i>continued</i> ) |                                                                                                              |         |
| <b>Co = 58.9332</b>                |                                                                                                              |         |
| 0.20965                            | $\text{Co} \leftrightarrow \text{CoSO}_4 \cdot 7\text{H}_2\text{O}$                                          | 4.7698  |
| 7.6743                             | $\text{K}_3[\text{Co}(\text{NO}_2)_6] \leftrightarrow \text{Co}$                                             | 0.13030 |
| 6.0357                             | $\text{K}_3[\text{Co}(\text{NO}_2)_6] \leftrightarrow \text{CoO}$                                            | 0.16568 |
| 1.3620                             | $\text{Co}_3\text{O}_4 \leftrightarrow \text{Co}$                                                            | 0.73422 |
| 1.0712                             | $\text{Co}_3\text{O}_4 \leftrightarrow \text{CoO}$                                                           | 0.93355 |
| 2.4758                             | $\text{Co}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Co}$                                                  | 0.40391 |
| 1.9471                             | $\text{Co}_2\text{P}_2\text{O}_7 \leftrightarrow \text{CoO}$                                                 | 0.51357 |
| 3.2233                             | $\text{CoNH}_4\text{PO}_4 \cdot \text{H}_2\text{O} \leftrightarrow \text{Co}$                                | 0.31024 |
| 2.5351                             | $\text{CoNH}_4\text{PO}_4 \cdot \text{H}_2\text{O} \leftrightarrow \text{CoO}$                               | 0.39447 |
| 2.6299                             | $\text{CoSO}_4 \leftrightarrow \text{Co}$                                                                    | 0.38024 |
| 2.0684                             | $\text{CoSO}_4 \leftrightarrow \text{CoO}$                                                                   | 0.48347 |
| 3.7514                             | $\text{CoSO}_4 \cdot 7\text{H}_2\text{O} \leftrightarrow \text{CoO}$                                         | 0.26657 |
| 7.0656                             | $(\text{CoSO}_4)_2 \cdot (\text{K}_2\text{SO}_4)_3 \leftrightarrow \text{Co}$                                | 0.14153 |
| 5.5569                             | $(\text{CoSO}_4)_2 \cdot (\text{K}_2\text{SO}_4)_3 \leftrightarrow \text{CoO}$                               | 0.17996 |
| <b>COPPER</b>                      |                                                                                                              |         |
| <b>Cu = 63.544</b>                 |                                                                                                              |         |
| 0.25071                            | $\text{Cu} \leftrightarrow \text{Cu}_2\text{C}_2\text{H}_3\text{O}_2 \cdot (\text{AsO}_2)_3$                 | 3.9887  |
| 0.79885                            | $\text{Cu} \leftrightarrow \text{CuO}$                                                                       | 1.2518  |
| 0.25449                            | $\text{Cu} \leftrightarrow \text{CuSO}_4 \cdot 5\text{H}_2\text{O}$                                          | 3.9295  |
| 1.9141                             | $\text{CuSCN} \leftrightarrow \text{Cu}$                                                                     | 0.52245 |
| 1.5291                             | $\text{CuSCN} \leftrightarrow \text{CuO}$                                                                    | 0.65400 |
| 0.31856                            | $\text{CuO} \leftrightarrow \text{CuSO}_4 \cdot 5\text{H}_2\text{O}$                                         | 3.1391  |
| 1.1259                             | $\text{Cu}_2\text{O} \leftrightarrow \text{Cu}$                                                              | 0.88817 |
| 1.2523                             | $\text{Cu}_2\text{S} \leftrightarrow \text{Cu}$                                                              | 0.79854 |
| 1.0004                             | $\text{Cu}_2\text{S} \leftrightarrow \text{CuO}$                                                             | 0.99961 |
| 1.1122                             | $\text{Cu}_2\text{S} \leftrightarrow \text{Cu}_2\text{O}$                                                    | 0.89908 |
| 0.31869                            | $\text{Cu}_2\text{S} \leftrightarrow \text{CuSO}_4 \cdot 5\text{H}_2\text{O}$                                | 3.1379  |
| 0.91872                            | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{Cu}_2\text{C}_2\text{H}_3\text{O}_2(\text{AsO}_2)_3$ | 1.0885  |
| <b>ERBIUM</b>                      |                                                                                                              |         |
| <b>Er = 167.26</b>                 |                                                                                                              |         |
| 1.1435                             | $\text{Er}_2\text{O}_3 \leftrightarrow \text{Er}$                                                            | 0.87452 |
| <b>FLUORINE</b>                    |                                                                                                              |         |
| <b>F = 18.9984</b>                 |                                                                                                              |         |
| 1.5936                             | $\text{BaSiF}_6 \leftrightarrow \text{BaF}_2$                                                                | 0.62751 |
| 2.4513                             | $\text{BaSiF}_6 \leftrightarrow \text{F}$                                                                    | 0.40795 |
| 2.3277                             | $\text{BaSiF}_6 \leftrightarrow 6\text{HF}$                                                                  | 0.42960 |
| 1.9392                             | $\text{BaSiF}_6 \leftrightarrow \text{H}_2\text{SiF}_6$                                                      | 0.51568 |
| 2.6847                             | $\text{BaSiF}_6 \leftrightarrow \text{SiF}_4$                                                                | 0.37249 |
| 1.9666                             | $\text{BaSiF}_6 \leftrightarrow \text{SiF}_6$                                                                | 0.50848 |
| 1.6256                             | $\text{CaF}_2 \leftrightarrow \text{H}_2\text{SiF}_6$                                                        | 0.61516 |
| 1.6486                             | $\text{CaF}_2 \leftrightarrow \text{SiF}_6$                                                                  | 0.60658 |
| 3.5829                             | $\text{CaSO}_4 \leftrightarrow \text{F}$                                                                     | 0.27910 |
| 2.4024                             | $\text{CaSO}_4 \leftrightarrow \text{HF}$                                                                    | 0.29391 |
| 0.48666                            | $\text{F} \leftrightarrow \text{CaF}_2$                                                                      | 2.0548  |
| 0.51248                            | $\text{HF} \leftrightarrow \text{CaF}_2$                                                                     | 1.9513  |
| 1.2641                             | $\text{H}_2\text{SiF}_6 \leftrightarrow \text{F}$                                                            | 0.79109 |
| 3.6011                             | $\text{H}_2\text{SiF}_6 \leftrightarrow 2\text{HF}$                                                          | 0.27769 |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                      |                                                                                              | Factor  |
|-----------------------------|----------------------------------------------------------------------------------------------|---------|
| <b>FLUORINE (continued)</b> |                                                                                              |         |
| <b>F = 18.9984</b>          |                                                                                              |         |
| 1.2004                      | $\text{H}_2\text{SiF}_6 \leftrightarrow 6\text{HF}$                                          | 0.83308 |
| 1.3844                      | $\text{H}_2\text{SiF}_6 \leftrightarrow \text{SiF}_4$                                        | 0.72233 |
| 1.0141                      | $\text{H}_2\text{SiF}_6 \leftrightarrow \text{SiF}_6$                                        | 0.98605 |
| 2.0556                      | $\text{KF} \cdot \text{HF} \leftrightarrow 2\text{F}$                                        | 0.48647 |
| 1.9520                      | $\text{KF} \cdot \text{HF} \leftrightarrow 2\text{HF}$                                       | 0.51228 |
| 0.67218                     | $\text{KF} \cdot \text{HF} \leftrightarrow 2\text{KF}$                                       | 1.4877  |
| 0.41489                     | $\text{KF} \cdot \text{HF} \leftrightarrow 2(\text{KF} \cdot 2\text{H}_2\text{O})$           | 2.4103  |
| 1.9325                      | $\text{K}_2\text{SiF}_6 \leftrightarrow \text{F}$                                            | 0.51748 |
| 1.8351                      | $\text{K}_2\text{SiF}_6 \leftrightarrow 6\text{HF}$                                          | 0.54494 |
| 1.5288                      | $\text{K}_2\text{SiF}_6 \leftrightarrow \text{H}_2\text{SiF}_6$                              | 0.65412 |
| 1.8957                      | $\text{K}_2\text{SiF}_6 \leftrightarrow 2\text{KF}$                                          | 0.52751 |
| 1.5504                      | $\text{K}_2\text{SiF}_6 \leftrightarrow \text{SiF}_6$                                        | 0.64500 |
| 1.9495                      | $\text{NH}_4\text{F} \leftrightarrow \text{F}$                                               | 0.51295 |
| 1.5013                      | $\text{NH}_4\text{F} \cdot \text{HF} \leftrightarrow 2\text{F}$                              | 0.66611 |
| 1.4256                      | $\text{NH}_4\text{F} \cdot \text{HF} \leftrightarrow 2\text{HF}$                             | 0.70145 |
| 0.49090                     | $\text{NH}_4\text{F} \cdot \text{HF} \leftrightarrow 2\text{KF}$                             | 2.0371  |
| 0.30300                     | $\text{NH}_4\text{F} \cdot \text{HF} \leftrightarrow 2(\text{KF} \cdot 2\text{H}_2\text{O})$ | 3.3003  |
| 1.5629                      | $(\text{NH}_4)_2\text{SiF}_6 \leftrightarrow \text{F}$                                       | 0.63985 |
| 1.4841                      | $(\text{NH}_4)_2\text{SiF}_6 \leftrightarrow 6\text{HF}$                                     | 0.67381 |
| 1.2364                      | $(\text{NH}_4)_2\text{SiF}_6 \leftrightarrow \text{H}_2\text{SiF}_6$                         | 0.80881 |
| 2.4050                      | $(\text{NH}_4)_2\text{SiF}_6 \leftrightarrow 2\text{NH}_4\text{F}$                           | 0.41580 |
| 1.2539                      | $(\text{NH}_4)_2\text{SiF}_6 \leftrightarrow \text{SiF}_6$                                   | 0.79753 |
| 2.2101                      | $\text{NaF} \leftrightarrow \text{F}$                                                        | 0.45246 |
| 1.6498                      | $\text{Na}_2\text{SiF}_6 \leftrightarrow \text{F}$                                           | 0.60614 |
| 1.5666                      | $\text{Na}_2\text{SiF}_6 \leftrightarrow 6\text{HF}$                                         | 0.63831 |
| 1.3052                      | $\text{Na}_3\text{SiF}_6 \leftrightarrow \text{H}_2\text{SiF}_6$                             | 0.76619 |
| 2.2394                      | $\text{Na}_2\text{SiF}_6 \leftrightarrow 2\text{NaF}$                                        | 0.44654 |
| 1.3236                      | $\text{Na}_2\text{SiF}_6 \leftrightarrow \text{SiF}_6$                                       | 0.75550 |
| <b>GALLIUM</b>              |                                                                                              |         |
| <b>Ga = 69.72</b>           |                                                                                              |         |
| 1.3442                      | $\text{Ga}_2\text{O}_3 \leftrightarrow \text{Ga}$                                            | 0.74392 |
| 1.6898                      | $\text{Ga}_2\text{S}_3 \leftrightarrow \text{Ga}$                                            | 0.59178 |
| <b>GERMANIUM</b>            |                                                                                              |         |
| <b>Ge = 72.59</b>           |                                                                                              |         |
| 1.4408                      | $\text{GeO}_2 \leftrightarrow \text{Ge}$                                                     | 0.69404 |
| 3.6476                      | $\text{K}_2\text{GeF}_6 \leftrightarrow \text{Ge}$                                           | 0.27415 |
| <b>GOLD</b>                 |                                                                                              |         |
| <b>Au = 196.967</b>         |                                                                                              |         |
| 0.64936                     | $\text{Au} \leftrightarrow \text{AuCl}_3$                                                    | 1.5400  |
| 0.47826                     | $\text{Au} \leftrightarrow \text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$                         | 2.0909  |
| 0.54995                     | $\text{Au} \leftrightarrow \text{KAu}(\text{CN})_4 \cdot \text{H}_2\text{O}$                 | 1.8183  |
| <b>HYDROGEN</b>             |                                                                                              |         |
| <b>H = 1.0079</b>           |                                                                                              |         |
| 8.9365                      | $\text{H}_2\text{O} \leftrightarrow \text{H}$                                                | 0.11190 |
| 7.9364                      | $\text{O} \leftrightarrow \text{H}$                                                          | 0.12600 |
| 0.35607                     | $\text{HSCN} \leftrightarrow \text{AgSCN}$                                                   | 2.8084  |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                      |                                                                                                      | Factor  |
|-----------------------------|------------------------------------------------------------------------------------------------------|---------|
| <b>HYDROGEN (continued)</b> |                                                                                                      |         |
| <b>H = 1.0079</b>           |                                                                                                      |         |
| 0.48586                     | $\text{HSCN} \leftrightarrow \text{CuSCN}$                                                           | 2.0582  |
| 0.25317                     | $\text{HSCN} \leftrightarrow \text{BaSO}_4$                                                          | 3.9499  |
| <b>INDIUM</b>               |                                                                                                      |         |
| <b>In = 114.82</b>          |                                                                                                      |         |
| 1.2090                      | $\text{In}_2\text{O}_3 \leftrightarrow \text{In}$                                                    | 0.82711 |
| 1.4189                      | $\text{In}_2\text{S}_3 \leftrightarrow \text{In}$                                                    | 0.70476 |
| <b>IODINE</b>               |                                                                                                      |         |
| <b>I = 126.904</b>          |                                                                                                      |         |
| 0.84333                     | $\text{Ag} \leftrightarrow \text{HI}$                                                                | 1.1858  |
| 0.85004                     | $\text{Ag} \leftrightarrow \text{I}$                                                                 | 1.1764  |
| 1.1294                      | $\text{AgCl} \leftrightarrow \text{I}$                                                               | 0.88543 |
| 1.8354                      | $\text{AgI} \leftrightarrow \text{HI}$                                                               | 0.54483 |
| 1.8500                      | $\text{AgI} \leftrightarrow \text{I}$                                                                | 0.54053 |
| 1.3423                      | $\text{AgI} \leftrightarrow \text{IO}_3$                                                             | 0.74498 |
| 1.2298                      | $\text{AgI} \leftrightarrow \text{IO}_4$                                                             | 0.81314 |
| 1.4066                      | $\text{AgI} \leftrightarrow \text{I}_2\text{O}_5$                                                    | 0.71091 |
| 1.2836                      | $\text{AgI} \leftrightarrow \text{I}_2\text{O}_7$                                                    | 0.77904 |
| 0.41592                     | $\text{Pd} \leftrightarrow \text{HI}$                                                                | 2.4043  |
| 0.41921                     | $\text{Pd} \leftrightarrow \text{I}$                                                                 | 2.3854  |
| 1.4081                      | $\text{PdI}_2 \leftrightarrow \text{HI}$                                                             | 0.71020 |
| 1.4192                      | $\text{PdI}_2 \leftrightarrow \text{I}$                                                              | 0.70462 |
| 1.0297                      | $\text{PdI}_2 \leftrightarrow \text{IO}_3$                                                           | 0.97113 |
| 0.94343                     | $\text{PdI}_2 \leftrightarrow \text{IO}_4$                                                           | 1.0600  |
| 1.0791                      | $\text{PdI}_2 \leftrightarrow \text{I}_2\text{O}_5$                                                  | 0.92671 |
| 0.98472                     | $\text{PdI}_2 \leftrightarrow \text{I}_2\text{O}_7$                                                  | 1.0155  |
| 2.5899                      | $\text{TlI} \leftrightarrow \text{HI}$                                                               | 0.38612 |
| 2.6105                      | $\text{TlI} \leftrightarrow \text{I}$                                                                | 0.38307 |
| 1.8941                      | $\text{TlI} \leftrightarrow \text{IO}_3$                                                             | 0.52797 |
| 1.7353                      | $\text{TlI} \leftrightarrow \text{IO}_4$                                                             | 0.57627 |
| 1.9848                      | $\text{TlI} \leftrightarrow \text{I}_2\text{O}_5$                                                    | 0.50383 |
| 1.8112                      | $\text{TlI} \leftrightarrow \text{I}_2\text{O}_7$                                                    | 0.55211 |
| <b>IRON</b>                 |                                                                                                      |         |
| <b>Fe = 55.845</b>          |                                                                                                      |         |
| 2.2598                      | $\text{Ag} \leftrightarrow \text{Fe}_7(\text{CN})_{18}$ (Prussian blue)                              | 0.44252 |
| 0.54503                     | $\text{CN} \leftrightarrow \text{Fe}_7(\text{CN})_{18}$                                              | 1.8347  |
| 0.61256                     | $\text{CO}_2 \leftrightarrow \text{FeO}$                                                             | 1.6325  |
| 0.37986                     | $\text{CO}_2 \leftrightarrow \text{FeCO}_3$                                                          | 2.6326  |
| 0.49483                     | $\text{CO}_2 \leftrightarrow \text{Fe}(\text{HCO}_3)_2$                                              | 2.0209  |
| 0.31396                     | $\text{Fe} \leftrightarrow \text{Fe}(\text{HCO}_3)_2$                                                | 3.1851  |
| 0.44061                     | $\text{Fe} \leftrightarrow \text{FeCl}_2$                                                            | 2.2696  |
| 0.77730                     | $\text{Fe} \leftrightarrow \text{FeO}$                                                               | 1.2865  |
| 0.69943                     | $\text{Fe} \leftrightarrow \text{Fe}_2\text{O}_3$                                                    | 1.4297  |
| 0.72359                     | $\text{Fe} \leftrightarrow \text{Fe}_3\text{O}_4$                                                    | 1.3820  |
| 0.36763                     | $\text{Fe} \leftrightarrow \text{FeSO}_4$                                                            | 2.7201  |
| 0.20087                     | $\text{Fe} \leftrightarrow \text{FeSO}_4 \cdot 7\text{H}_2\text{O}$                                  | 4.9782  |
| 0.14242                     | $\text{Fe} \leftrightarrow \text{FeSO}_4 \cdot (\text{NH}_4)_2\text{SO}_4 \cdot 6\text{H}_2\text{O}$ | 7.0217  |
| 0.62011                     | $\text{FeO} \leftrightarrow \text{FeCO}_3$                                                           | 1.6126  |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                  |                                                                                                                  | Factor   |
|-------------------------|------------------------------------------------------------------------------------------------------------------|----------|
| <b>IRON (continued)</b> |                                                                                                                  |          |
| <b>Fe = 55.845</b>      |                                                                                                                  |          |
| 0.40390                 | $\text{FeO} \leftrightarrow \text{Fe}(\text{HCO}_3)_2$                                                           | 2.4759   |
| 0.89982                 | $\text{FeO} \leftrightarrow \text{Fe}_2\text{O}_3$                                                               | 1.1113   |
| 0.49223                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FeCl}_2$                                                            | 2.0316   |
| 0.68915                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FeCO}_3$                                                            | 1.4511   |
| 0.44887                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{Fe}(\text{HCO}_3)_2$                                                | 2.2278   |
| 0.33422                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{Fe}(\text{HCO}_3)_3$                                                | 2.9920   |
| 1.1113                  | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FeO}$                                                               | 0.89982  |
| 1.0345                  | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{Fe}_3\text{O}_4$                                                    | 0.96662  |
| 0.52941                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FePO}_4$                                                            | 1.8889   |
| 0.52561                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FeSO}_4$                                                            | 1.9026   |
| 0.28719                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FeSO}_4 \cdot 7\text{H}_2\text{O}$                                  | 3.4820   |
| 0.20361                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{FeSO}_4 \cdot (\text{NH}_4)_2\text{SO}_4 \cdot 6\text{H}_2\text{O}$ | 4.9113   |
| 0.39934                 | $\text{Fe}_2\text{O}_3 \leftrightarrow \text{Fe}_2(\text{SO}_4)_3$                                               | 2.5041   |
| 2.7006                  | $\text{FePO}_4 \leftrightarrow \text{Fe}$                                                                        | 0.37029  |
| 2.0992                  | $\text{FePO}_4 \leftrightarrow \text{FeO}$                                                                       | 0.47637  |
| 1.5741                  | $\text{FeS} \leftrightarrow \text{Fe}$                                                                           | 0.63527  |
| 1.2236                  | $\text{FeS} \leftrightarrow \text{FeO}$                                                                          | 0.81726  |
| 1.1010                  | $\text{FeS} \leftrightarrow \text{Fe}_2\text{O}_3$                                                               | 0.90825  |
| 0.79699                 | $\text{Mg}_2\text{As}_2\text{O}_7 \leftrightarrow \text{FeAsO}_4$                                                | 1.2547   |
| 1.1144                  | $\text{SO}_3 \leftrightarrow \text{FeO}$                                                                         | 0.89738  |
| 0.52704                 | $\text{SO}_3 \leftrightarrow \text{FeSO}_4$                                                                      | 1.8974   |
| <b>LANTHANUM</b>        |                                                                                                                  |          |
| <b>La = 138.91</b>      |                                                                                                                  |          |
| 1.1728                  | $\text{La}_2\text{O}_3 \leftrightarrow \text{La}$                                                                | 0.85268  |
| <b>LEAD</b>             |                                                                                                                  |          |
| <b>Pb = 207.2</b>       |                                                                                                                  |          |
| 0.77541                 | $\text{Pb} \leftrightarrow \text{PbCO}_3$                                                                        | 1.2896   |
| 0.80141                 | $\text{Pb} \leftrightarrow (\text{PbCO}_3)_2 \cdot \text{Pb}(\text{OH})_2$                                       | 1.2478   |
| 0.85901                 | $\text{Pb} \leftrightarrow \text{Pb}(\text{OH})_2$                                                               | 1.1641   |
| 0.92831                 | $\text{Pb} \leftrightarrow \text{PbO}$                                                                           | 1.0772   |
| 1.3422                  | $\text{PbCl}_2 \leftrightarrow \text{Pb}$                                                                        | 0.74502  |
| 1.2460                  | $\text{PbCl}_2 \leftrightarrow \text{PbO}$                                                                       | 0.80255  |
| 1.5598                  | $\text{PbCrO}_4 \leftrightarrow \text{Pb}$                                                                       | 0.641110 |
| 0.85198                 | $\text{PbCrO}_4 \leftrightarrow \text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$           | 1.1737   |
| 1.2501                  | $\text{PbCrO}_4 \leftrightarrow (\text{PbCO}_3)_2 \cdot \text{Pb}(\text{OH})_2$                                  | 0.79997  |
| 1.4480                  | $\text{PbCrO}_4 \leftrightarrow \text{PbO}$                                                                      | 0.69061  |
| 1.4142                  | $\text{PbCrO}_4 \leftrightarrow \text{Pb}_3\text{O}_4$                                                           | 0.70711  |
| 1.0657                  | $\text{PbCrO}_4 \leftrightarrow \text{PbSO}_4$                                                                   | 0.93833  |
| 0.83529                 | $\text{PbO} \leftrightarrow \text{PbCO}_3$                                                                       | 1.1972   |
| 0.67388                 | $\text{PbO} \leftrightarrow \text{Pb}(\text{NO}_3)_2$                                                            | 1.4839   |
| 0.93311                 | $\text{PbO} \leftrightarrow \text{PbO}_2$                                                                        | 1.0717   |
| 1.1544                  | $\text{PbO}_2 \leftrightarrow \text{Pb}$                                                                         | 0.86622  |
| 0.72219                 | $\text{PbO}_2 \leftrightarrow \text{Pb}(\text{NO}_3)_2$                                                          | 1.3847   |
| 1.1547                  | $\text{PbS} \leftrightarrow \text{Pb}$                                                                           | 0.86600  |
| 1.0720                  | $\text{PbS} \leftrightarrow \text{PbO}$                                                                          | 0.93287  |
| 0.78895                 | $\text{PbS} \leftrightarrow \text{PbSO}_4$                                                                       | 1.2675   |
| 1.2993                  | $\text{PbSO}_4 \leftrightarrow \text{BaSO}_4$                                                                    | 0.76966  |
| 1.4636                  | $\text{PbSO}_4 \leftrightarrow \text{Pb}$                                                                        | 0.68323  |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                  |                                                                                                       | Factor   |
|-------------------------|-------------------------------------------------------------------------------------------------------|----------|
| <b>LEAD (continued)</b> |                                                                                                       |          |
| <b>Pb = 207.2</b>       |                                                                                                       |          |
| 0.79944                 | $\text{PbSO}_4 \leftrightarrow \text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$ | 1.2509   |
| 1.1349                  | $\text{PbSO}_4 \leftrightarrow \text{PbCO}_3$                                                         | 0.88112  |
| 1.1730                  | $\text{PbSO}_4 \leftrightarrow (\text{PbCO}_3)_2 \cdot \text{Pb}(\text{OH})_2$                        | 0.85254  |
| 0.91561                 | $\text{PbSO}_4 \leftrightarrow \text{Pb}(\text{NO}_3)_2$                                              | 1.0922   |
| 1.3587                  | $\text{PbSO}_4 \leftrightarrow \text{PbO}$                                                            | 0.73599  |
| 1.2678                  | $\text{PbSO}_4 \leftrightarrow \text{PbO}_2$                                                          | 0.78875  |
| 1.3270                  | $\text{PbSO}_4 \leftrightarrow \text{Pb}_3\text{O}_4$                                                 | 0.75358  |
| <b>LITHIUM</b>          |                                                                                                       |          |
| <b>Li = 6.941</b>       |                                                                                                       |          |
| 0.59562                 | $\text{CO}_2 \leftrightarrow \text{Li}_2\text{CO}_3$                                                  | 1.6789   |
| 0.64759                 | $\text{CO}_2 \leftrightarrow \text{LiHCO}_3$                                                          | 1.5442   |
| 1.4729                  | $\text{CO}_2 \leftrightarrow \text{Li}_2\text{O}$                                                     | 0.67894  |
| 6.1086                  | $\text{LiCl} \leftrightarrow \text{Li}$                                                               | 0.16369  |
| 2.8378                  | $\text{LiCl} \leftrightarrow \text{Li}_2\text{O}$                                                     | 0.35239  |
| 5.3228                  | $\text{Li}_2\text{CO}_3 \leftrightarrow \text{Li}$                                                    | 0.18787  |
| 0.87147                 | $\text{Li}_2\text{CO}_3 \leftrightarrow \text{LiCl}$                                                  | 1.1475   |
| 0.54364                 | $\text{Li}_2\text{CO}_3 \leftrightarrow \text{LiHCO}_3$                                               | 1.8395   |
| 2.4730                  | $\text{Li}_2\text{CO}_3 \leftrightarrow \text{Li}_2\text{O}$                                          | 0.40436  |
| 4.5491                  | $\text{LiHCO}_3 \leftrightarrow \text{Li}_2\text{O}$                                                  | 0.21983  |
| 3.7371                  | $\text{LiF} \leftrightarrow \text{Li}$                                                                | 0.26759  |
| 2.1525                  | $\text{Li}_2\text{O} \leftrightarrow \text{Li}$                                                       | 0.46457  |
| 0.27176                 | $\text{Li}_2\text{O} \leftrightarrow \text{Li}_2\text{SO}_4$                                          | 3.6798   |
| 5.5609                  | $\text{Li}_2\text{PO}_4 \leftrightarrow \text{Li}$                                                    | 0.17983  |
| 0.91047                 | $\text{Li}_3\text{PO}_4 \leftrightarrow \text{LiCl}$                                                  | 1.0983   |
| 1.0447                  | $\text{Li}_3\text{PO}_4 \leftrightarrow \text{Li}_2\text{CO}_3$                                       | 0.95717  |
| 0.56797                 | $\text{Li}_3\text{PO}_4 \leftrightarrow \text{LiHCO}_3$                                               | 1.7607   |
| 2.5837                  | $\text{Li}_3\text{PO}_4 \leftrightarrow \text{Li}_2\text{O}$                                          | 0.38704  |
| 0.70214                 | $\text{Li}_3\text{PO}_4 \leftrightarrow \text{Li}_2\text{SO}_4$                                       | 1.4242   |
| 0.60331                 | $\text{Li}_3\text{PO}_4 \leftrightarrow \text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$              | 1.6575   |
| 7.9153                  | $\text{Li}_2\text{SO}_4 \leftrightarrow \text{Li}$                                                    | 0.12634  |
| 1.2967                  | $\text{Li}_2\text{SO}_4 \leftrightarrow \text{LiCl}$                                                  | 0.77118  |
| 2.6797                  | $\text{SO}_3 \leftrightarrow \text{Li}_2\text{O}$                                                     | 0.37317  |
| 0.72823                 | $\text{SO}_3 \leftrightarrow \text{Li}_2\text{SO}_4$                                                  | 1.3732   |
| <b>MAGNESIUM</b>        |                                                                                                       |          |
| <b>Mg = 24.305</b>      |                                                                                                       |          |
| 1.9390                  | $\text{BaSO}_4 \leftrightarrow \text{MgSO}_4$                                                         | 0.51572  |
| 0.94693                 | $\text{BaSO}_4 \leftrightarrow \text{MgSO}_4 \cdot 7\text{H}_2\text{O}$                               | 1.0560   |
| 6.5755                  | $\text{Br} \leftrightarrow \text{Mg}$                                                                 | 0.15208  |
| 0.86800                 | $\text{Br} \leftrightarrow \text{MgBr}_2$                                                             | 1.1521   |
| 0.54691                 | $\text{Br} \leftrightarrow \text{MgBr}_2 \cdot 6\text{H}_2\text{O}$                                   | 1.8285   |
| 2.9173                  | $\text{Cl} \leftrightarrow \text{Mg}$                                                                 | 0.34278  |
| 0.74472                 | $\text{Cl} \leftrightarrow \text{MgCl}_2$                                                             | 1.3429   |
| 0.25533                 | $\text{Mg} \leftrightarrow \text{MgCl}_2$                                                             | 3.9165   |
| 0.28883                 | $\text{Mg} \leftrightarrow \text{MgCO}_3$                                                             | 3.4683   |
| 10.4427                 | $\text{I} \leftrightarrow \text{Mg}$                                                                  | 0.095761 |
| 0.91261                 | $\text{I} \leftrightarrow \text{MgI}_2$                                                               | 1.09576  |
| 0.34876                 | $\text{Cl} \leftrightarrow \text{MgCl}_2 \cdot 6\text{H}_2\text{O}$                                   | 2.8673   |
| 0.52193                 | $\text{CO}_2 \leftrightarrow \text{MgCO}_3$                                                           | 1.9160   |



TABLE 11.19 Gravimetric Factors (Continued)

| Factor                       |                                                                                                            | Factor   |
|------------------------------|------------------------------------------------------------------------------------------------------------|----------|
| <b>MAGNESIUM</b> (continued) |                                                                                                            |          |
| <b>Mg = 24.305</b>           |                                                                                                            |          |
| 1.0918                       | $\text{CO}_2 \leftrightarrow \text{MgO}$                                                                   | 0.91595  |
| 0.57616                      | $\text{MgCO}_3 \leftrightarrow \text{Mg}(\text{HCO}_3)_2$                                                  | 1.7356   |
| 10.094                       | $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O} \leftrightarrow \text{Mg}$                             | 0.099067 |
| 6.0879                       | $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O} \leftrightarrow \text{MgO}$                            | 0.16426  |
| 1.6581                       | $\text{MgO} \leftrightarrow \text{Mg}$                                                                     | 0.60311  |
| 0.47807                      | $\text{MgO} \leftrightarrow \text{MgCO}_3$                                                                 | 2.0918   |
| 0.27544                      | $\text{MgO} \leftrightarrow \text{Mg}(\text{HCO}_3)_2$                                                     | 3.6305   |
| 0.33489                      | $\text{MgO} \leftrightarrow \text{MgSO}_4$                                                                 | 2.9860   |
| 4.5784                       | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Mg}$                                                | 0.21841  |
| 1.1687                       | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgCl}_2$                                            | 0.85562  |
| 0.54737                      | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgCl}_2 \cdot 6\text{H}_2\text{O}$                  | 1.8269   |
| 0.40049                      | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgCl}_2 \cdot \text{KCl} \cdot 6\text{H}_2\text{O}$ | 2.4969   |
| 1.3198                       | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgCO}_3$                                            | 0.75770  |
| 0.76040                      | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Mg}(\text{HCO}_3)_2$                                | 1.3151   |
| 2.7607                       | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgO}$                                               | 0.36223  |
| 0.92452                      | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgSO}_4$                                            | 1.0816   |
| 0.45150                      | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MgSO}_4 \cdot 7\text{H}_2\text{O}$                  | 2.2149   |
| 4.9523                       | $\text{MgSO}_4 \leftrightarrow \text{Mg}$                                                                  | 0.20193  |
| 1.9864                       | $\text{SO}_3 \leftrightarrow \text{MgO}$                                                                   | 0.50343  |
| 0.6651                       | $\text{SO}_3 \leftrightarrow \text{MgSO}_4$                                                                | 1.5034   |
| 0.38482                      | $\text{SO}_3 \leftrightarrow \text{MgSO}_4 \cdot 7\text{H}_2\text{O}$                                      | 3.0786   |
| <b>MANGANESE</b>             |                                                                                                            |          |
| <b>Mn = 54.9380</b>          |                                                                                                            |          |
| 1.5457                       | $\text{BaSO}_4 \leftrightarrow \text{MnSO}_4$                                                              | 0.64696  |
| 0.38286                      | $\text{CO}_2 \leftrightarrow \text{MnCO}_3$                                                                | 2.6119   |
| 0.62041                      | $\text{CO}_2 \leftrightarrow \text{MnO}$                                                                   | 1.6118   |
| 0.47793                      | $\text{Mn} \leftrightarrow \text{MnCO}_3$                                                                  | 2.0924   |
| 0.77446                      | $\text{Mn} \leftrightarrow \text{MnO}$                                                                     | 1.2912   |
| 0.63193                      | $\text{Mn} \leftrightarrow \text{MnO}_2$                                                                   | 1.5825   |
| 0.69599                      | $\text{Mn} \leftrightarrow \text{Mn}_2\text{O}_3$                                                          | 1.4368   |
| 0.76126                      | $\text{MnCO}_3 \leftrightarrow \text{MnSO}_4$                                                              | 1.3136   |
| 1.5395                       | $\text{Mn}(\text{HCO}_3)_2 \leftrightarrow \text{MnCO}_3$                                                  | 0.64955  |
| 0.61711                      | $\text{MnO} \leftrightarrow \text{MnCO}_3$                                                                 | 1.6205   |
| 0.40084                      | $\text{MnO} \leftrightarrow \text{Mn}(\text{HCO}_3)_2$                                                     | 2.4947   |
| 0.89868                      | $\text{MnO} \leftrightarrow \text{Mn}_2\text{O}_3$                                                         | 1.1127   |
| 0.46978                      | $\text{MnO} \leftrightarrow \text{MnSO}_4$                                                                 | 2.1286   |
| 1.3883                       | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{Mn}$                                                          | 0.72031  |
| 0.66351                      | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{MnCO}_3$                                                      | 1.5071   |
| 0.43098                      | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{Mn}(\text{HCO}_3)_2$                                          | 2.3203   |
| 1.0752                       | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{MnO}$                                                         | 0.93008  |
| 0.96625                      | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{Mn}_2\text{O}_3$                                              | 1.0349   |
| 0.87731                      | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{MnO}_2$                                                       | 1.1399   |
| 0.50510                      | $\text{Mn}_3\text{O}_4 \leftrightarrow \text{MnSO}_4$                                                      | 1.9798   |
| 2.5831                       | $\text{Mn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Mn}$                                                | 0.38713  |
| 1.2345                       | $\text{Mn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MnCO}_3$                                            | 0.81002  |
| 2.0005                       | $\text{Mn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MnO}$                                               | 0.49987  |
| 1.6324                       | $\text{Mn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MnO}_2$                                             | 0.61261  |
| 0.93980                      | $\text{Mn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{MnSO}_4$                                            | 1.0641   |
| 1.5836                       | $\text{MnS} \leftrightarrow \text{Mn}$                                                                     | 0.63146  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                                |                                                                                               | Factor  |
|---------------------------------------|-----------------------------------------------------------------------------------------------|---------|
| <b>MANGANESE</b> ( <i>continued</i> ) |                                                                                               |         |
| <b>Mn = 54.9380</b>                   |                                                                                               |         |
| 0.75687                               | $\text{MnS} \leftrightarrow \text{MnCO}_3$                                                    | 1.3212  |
| 1.2265                                | $\text{MnS} \leftrightarrow \text{MnO}$                                                       | 0.81535 |
| 0.57617                               | $\text{MnS} \leftrightarrow \text{MnSO}_4$                                                    | 1.7356  |
| 2.7486                                | $\text{MnSO}_4 \leftrightarrow \text{Mn}$                                                     | 0.36383 |
| 1.1286                                | $\text{SO}_3 \leftrightarrow \text{MnO}$                                                      | 0.88603 |
| 0.53021                               | $\text{SO}_3 \leftrightarrow \text{MnSO}_4$                                                   | 1.8860  |
| <b>MERCURY</b>                        |                                                                                               |         |
| <b>Hg = 200.59</b>                    |                                                                                               |         |
| 0.73882                               | $\text{Hg} \leftrightarrow \text{HgCl}_2$                                                     | 1.3535  |
| 0.92613                               | $\text{Hg} \leftrightarrow \text{HgO}$                                                        | 1.0798  |
| 0.86220                               | $\text{Hg} \leftrightarrow \text{HgS}$                                                        | 1.1598  |
| 1.1767                                | $\text{HgCl} \leftrightarrow \text{Hg}$                                                       | 0.84981 |
| 0.86939                               | $\text{HgCl} \leftrightarrow \text{HgCl}_2$                                                   | 1.1502  |
| 0.89889                               | $\text{HgCl} \leftrightarrow \text{HgNO}_3$                                                   | 1.1125  |
| 1.1316                                | $\text{HgCl} \leftrightarrow \text{Hg}_2\text{O}$                                             | 0.88371 |
| 1.0898                                | $\text{HgCl} \leftrightarrow \text{HgO}$                                                      | 0.91760 |
| 1.0146                                | $\text{HgCl} \leftrightarrow \text{HgS}$                                                      | 0.98564 |
| 0.98564                               | $\text{HgS} \leftrightarrow \text{HgCl}$                                                      | 1.0146  |
| 0.85691                               | $\text{HgS} \leftrightarrow \text{HgCl}_2$                                                    | 1.1670  |
| 0.92091                               | $\text{HgS} \leftrightarrow \text{Hg}(\text{CN})_2$                                           | 1.0859  |
| 0.88598                               | $\text{HgS} \leftrightarrow \text{HgNO}_3$                                                    | 1.1287  |
| 0.71673                               | $\text{HgS} \leftrightarrow \text{Hg}(\text{NO}_3)_2$                                         | 1.3952  |
| 0.67903                               | $\text{HgS} \leftrightarrow \text{Hg}(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$                | 1.4727  |
| 1.1153                                | $\text{HgS} \leftrightarrow \text{Hg}_2\text{O}$                                              | 0.89658 |
| 1.0741                                | $\text{HgS} \leftrightarrow \text{HgO}$                                                       | 0.93097 |
| 0.78426                               | $\text{HgS} \leftrightarrow \text{HgSO}_4$                                                    | 1.2751  |
| <b>MOLYBDENUM</b>                     |                                                                                               |         |
| <b>Mo = 95.94</b>                     |                                                                                               |         |
| 8.9876                                | $\text{MoC} \leftrightarrow \text{C}$                                                         | 0.11126 |
| 1.5003                                | $\text{MoO}_3 \leftrightarrow \text{Mo}$                                                      | 0.66653 |
| 0.73436                               | $\text{MoO}_3 \leftrightarrow (\text{NH}_4)_2\text{MoO}_4$                                    | 1.3617  |
| 2.0026                                | $\text{MoS}_3 \leftrightarrow \text{Mo}$                                                      | 0.49935 |
| 1.3348                                | $\text{MoS}_4 \leftrightarrow \text{MoO}_3$                                                   | 0.74918 |
| 0.98021                               | $\text{MoS}_3 \leftrightarrow (\text{NH}_4)_2\text{MoO}_4$                                    | 1.0202  |
| 1.0863                                | $(\text{NH}_4)_3\text{PO}_4 \cdot 12\text{MoO}_3 \leftrightarrow \text{MoO}_3$                | 0.92058 |
| 0.79771                               | $(\text{NH}_4)_3\text{PO}_4 \cdot 12\text{MoO}_3 \leftrightarrow (\text{NH}_4)_2\text{MoO}_4$ | 1.2536  |
| 3.8267                                | $\text{PbMoO}_4 \leftrightarrow \text{Mo}$                                                    | 0.26132 |
| 2.5506                                | $\text{PbMoO}_4 \leftrightarrow \text{MoO}_3$                                                 | 0.39207 |
| 1.8730                                | $\text{PbMoO}_4 \leftrightarrow (\text{NH}_4)_2\text{MoO}_4$                                  | 0.53390 |
| <b>NEODYMIUM</b>                      |                                                                                               |         |
| <b>Nd = 144.24</b>                    |                                                                                               |         |
| 1.1664                                | $\text{Nd}_2\text{O}_3 \leftrightarrow \text{Nd}$                                             | 0.85735 |
| <b>NICKEL</b>                         |                                                                                               |         |
| <b>Ni = 58.71</b>                     |                                                                                               |         |
| 0.20319                               | $\text{Ni} \leftrightarrow \text{Ni dimethylglyoxime}$                                        | 4.9215  |
| 0.20188                               | $\text{Ni} \leftrightarrow \text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$                | 4.9533  |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                    |                                                                                    | Factor   |
|---------------------------|------------------------------------------------------------------------------------|----------|
| <b>NICKEL (continued)</b> |                                                                                    |          |
| <b>Ni = 58.71</b>         |                                                                                    |          |
| 0.78585                   | $\text{Ni} \leftrightarrow \text{NiO}$                                             | 1.2725   |
| 0.20902                   | $\text{Ni} \leftrightarrow \text{NiSO}_4 \cdot 7\text{H}_2\text{O}$                | 4.7842   |
| 3.8675                    | $\text{Ni dimethylglyoxime} \leftrightarrow \text{NiO}$                            | 0.25856  |
| 0.25690                   | $\text{NiO} \leftrightarrow \text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$    | 3.8926   |
| 0.26598                   | $\text{NiO} \leftrightarrow \text{NiSO}_4 \cdot 7\text{H}_2\text{O}$               | 3.7597   |
| 2.6362                    | $\text{NiSO}_4 \leftrightarrow \text{Ni}$                                          | 0.37934  |
| 0.53220                   | $\text{NiSO}_4 \leftrightarrow \text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ | 1.8790   |
| 2.0716                    | $\text{NiSO}_4 \leftrightarrow \text{NiO}$                                         | 0.48271  |
| 0.55102                   | $\text{NiSO}_4 \leftrightarrow \text{NiSO}_4 \cdot 7\text{H}_2\text{O}$            | 1.8148   |
| <b>NIOBIUM</b>            |                                                                                    |          |
| <b>Nb = 92.906</b>        |                                                                                    |          |
| 7.7351                    | $\text{Nb} \leftrightarrow \text{C}$                                               | 0.12928  |
| 8.7353                    | $\text{NbC} \leftrightarrow \text{C}$                                              | 0.11448  |
| 11.065                    | $\text{Nb}_2\text{O}_5 \leftrightarrow 2\text{C}$                                  | 0.090373 |
| 1.4305                    | $\text{Nb}_2\text{O}_5 \leftrightarrow \text{Nb}$                                  | 0.69904  |
| <b>NITROGEN</b>           |                                                                                    |          |
| <b>N = 14.0067</b>        |                                                                                    |          |
| 3.2731                    | $\text{AgNO}_2 \leftrightarrow \text{HNO}_2$                                       | 0.30552  |
| 4.0488                    | $\text{AgNO}_2 \leftrightarrow \text{N}_2\text{O}_3$                               | 0.24698  |
| 1.8722                    | $\text{KNO}_3 \leftrightarrow \text{N}_2\text{O}_5$                                | 0.53412  |
| 0.22229                   | $\text{N} \leftrightarrow \text{HNO}_3$                                            | 4.4987   |
| 0.30446                   | $\text{N} \leftrightarrow \text{NO}_2$                                             | 3.2845   |
| 0.36855                   | $\text{N} \leftrightarrow \text{N}_2\text{O}_3$                                    | 2.7134   |
| 0.22590                   | $\text{N} \leftrightarrow \text{NO}_3$                                             | 4.4268   |
| 0.25936                   | $\text{N} \leftrightarrow \text{N}_2\text{O}_5$                                    | 3.8556   |
| 6.0680                    | $\text{NaNO}_3 \leftrightarrow \text{N}$                                           | 0.16480  |
| 1.5738                    | $\text{NaNO}_3 \leftrightarrow \text{N}_2\text{O}_5$                               | 0.63539  |
| 0.47619                   | $\text{NO} \leftrightarrow \text{HNO}_3$                                           | 2.1000   |
| 0.65222                   | $\text{NO} \leftrightarrow \text{NO}_2$                                            | 1.5332   |
| 0.78951                   | $\text{NO} \leftrightarrow \text{N}_2\text{O}_3$                                   | 1.2666   |
| 0.48393                   | $\text{NO} \leftrightarrow \text{NO}_3$                                            | 2.0664   |
| 0.55561                   | $\text{NO} \leftrightarrow \text{N}_2\text{O}_5$                                   | 1.7998   |
| 0.27028                   | $\text{NH}_3 \leftrightarrow \text{HNO}_3$                                         | 3.6999   |
| 1.2159                    | $\text{NH}_3 \leftrightarrow \text{N}$                                             | 0.82244  |
| 0.31536                   | $\text{NH}_3 \leftrightarrow \text{N}_2\text{O}_5$                                 | 3.1710   |
| 0.27467                   | $\text{NH}_3 \leftrightarrow \text{NO}_3$                                          | 3.6407   |
| 0.84890                   | $\text{NH}_4\text{Cl} \leftrightarrow \text{HNO}_3$                                | 1.1780   |
| 0.86270                   | $\text{NH}_4\text{Cl} \leftrightarrow \text{NO}_3$                                 | 1.1591   |
| 0.99050                   | $\text{NH}_4\text{Cl} \leftrightarrow \text{N}_2\text{O}_5$                        | 1.0096   |
| 3.8189                    | $\text{NH}_4\text{Cl} \leftrightarrow \text{N}$                                    | 0.26185  |
| 3.5221                    | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{HNO}_3$                        | 0.28393  |
| 15.845                    | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{N}$                            | 0.063112 |
| 4.1096                    | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{N}_2\text{O}_6$                | 0.24333  |
| 3.5794                    | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{NO}_3$                         | 0.27938  |
| 4.7169                    | $(\text{NH}_4)_2\text{SO}_4 \leftrightarrow \text{N}$                              | 0.21200  |
| 1.2234                    | $(\text{NH}_4)_2\text{SO}_4 \leftrightarrow \text{N}_2\text{O}_5$                  | 0.81739  |
| 1.5480                    | $\text{Pt} \leftrightarrow \text{HNO}_3$                                           | 0.64599  |
| 6.9640                    | $\text{Pt} \leftrightarrow \text{N}$                                               | 0.14360  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                               |                                                                                                       | Factor   |
|--------------------------------------|-------------------------------------------------------------------------------------------------------|----------|
| <b>NITROGEN</b> ( <i>continued</i> ) |                                                                                                       |          |
| <b>N = 14.0067</b>                   |                                                                                                       |          |
| 1.5732                               | $\text{Pt} \leftrightarrow \text{NO}_3$                                                               | 0.63566  |
| 1.8062                               | $\text{Pt} \leftrightarrow \text{N}_2\text{O}_5$                                                      | 0.55364  |
| 0.63528                              | $\text{SO}_3 \leftrightarrow \text{HNO}_3$                                                            | 1.5741   |
| 2.8579                               | $\text{SO}_3 \leftrightarrow \text{N}$                                                                | 0.34990  |
| 0.74125                              | $\text{SO}_3 \leftrightarrow \text{N}_2\text{O}_5$                                                    | 1.3491   |
| <b>OSMIUM</b>                        |                                                                                                       |          |
| <b>Os = 190.2</b>                    |                                                                                                       |          |
| 1.3365                               | $\text{OsO}_4 \leftrightarrow \text{Os}$                                                              | 0.74823  |
| <b>PALLADIUM</b>                     |                                                                                                       |          |
| <b>Pd = 106.4</b>                    |                                                                                                       |          |
| 0.49873                              | $\text{Pd} \leftrightarrow \text{PdCl}_2 \cdot 2\text{H}_2\text{O}$                                   | 2.0051   |
| 0.46179                              | $\text{Pd} \leftrightarrow \text{Pd}(\text{NO}_3)_2$                                                  | 2.1655   |
| 3.3854                               | $\text{PdI}_2 \leftrightarrow \text{Pd}$                                                              | 0.29538  |
| 3.7342                               | $\text{K}_2\text{PdCl}_6 \leftrightarrow \text{Pd}$                                                   | 0.26779  |
| 1.8624                               | $\text{K}_2\text{PdCl}_6 \leftrightarrow \text{PdCl}_2 \cdot 2\text{H}_2\text{O}$                     | 0.53695  |
| <b>PHOSPHORUS</b>                    |                                                                                                       |          |
| <b>P = 30.9738</b>                   |                                                                                                       |          |
| 13.514                               | $\text{Ag}_3\text{PO}_4 \leftrightarrow \text{P}$                                                     | 0.073998 |
| 4.4075                               | $\text{Ag}_3\text{PO}_4 \leftrightarrow \text{PO}_4$                                                  | 0.22689  |
| 5.8980                               | $\text{Ag}_3\text{PO}_4 \leftrightarrow \text{P}_2\text{O}_5$                                         | 0.16955  |
| 9.7730                               | $\text{Ag}_4\text{P}_2\text{O}_7 \leftrightarrow \text{P}$                                            | 0.10232  |
| 3.1874                               | $\text{Ag}_4\text{P}_2\text{O}_7 \leftrightarrow \text{PO}_4$                                         | 0.31374  |
| 4.2653                               | $\text{Ag}_4\text{P}_2\text{O}_7 \leftrightarrow \text{P}_2\text{O}_5$                                | 0.23445  |
| 0.71833                              | $\text{Al}_2\text{O}_3 \leftrightarrow \text{P}_2\text{O}_5$                                          | 1.3921   |
| 1.2841                               | $\text{AlPO}_4 \leftrightarrow \text{PO}_4$                                                           | 0.77877  |
| 1.7183                               | $\text{AlPO}_4 \leftrightarrow \text{P}_2\text{O}_5$                                                  | 0.58196  |
| 2.1853                               | $\text{Ca}_3(\text{PO}_4)_2 \leftrightarrow \text{P}_2\text{O}_5$                                     | 0.45761  |
| 1.5881                               | $\text{FePO}_4 \leftrightarrow \text{PO}_4$                                                           | 0.62970  |
| 2.1251                               | $\text{FePO}_4 \leftrightarrow \text{P}_2\text{O}_5$                                                  | 0.47056  |
| 0.78392                              | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Na}_2\text{HPO}_4$                             | 1.2756   |
| 0.31073                              | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$  | 3.2182   |
| 0.53229                              | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{NaNH}_4\text{HPO}_4 \cdot 4\text{H}_2\text{O}$ | 1.8787   |
| 3.5929                               | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{P}$                                            | 0.27833  |
| 1.1718                               | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{PO}_4$                                         | 0.85340  |
| 1.5681                               | $\text{Mg}_2\text{P}_2\text{O}_7 \leftrightarrow \text{P}_2\text{O}_5$                                | 0.63773  |
| 60.577                               | $(\text{NH}_4)_3\text{PO}_4 \cdot 12\text{MoO}_3 \leftrightarrow \text{P}$                            | 0.016508 |
| 19.757                               | $(\text{NH}_4)_3\text{PO}_4 \cdot 12\text{MoO}_3 \leftrightarrow \text{PO}_4$                         | 0.050616 |
| 26.438                               | $(\text{NH}_4)_3\text{PO}_4 \cdot 12\text{MoO}_3 \leftrightarrow \text{P}_2\text{O}_5$                | 0.037824 |
| 0.63773                              | $\text{P}_2\text{O}_5 \leftrightarrow \text{Mg}_2\text{P}_2\text{O}_7$                                | 1.5681   |
| 0.49993                              | $\text{P}_2\text{O}_5 \leftrightarrow \text{Na}_2\text{HPO}_4$                                        | 2.0003   |
| 0.19816                              | $\text{P}_2\text{O}_5 \leftrightarrow \text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$             | 5.0464   |
| 0.33946                              | $\text{P}_2\text{O}_5 \leftrightarrow \text{NaNH}_4\text{HPO}_4 \cdot 4\text{H}_2\text{O}$            | 2.9459   |
| 2.2913                               | $\text{P}_2\text{O}_5 \leftrightarrow \text{P}$                                                       | 0.43644  |
| 58.057                               | $\text{P}_2\text{O}_5 \cdot 24\text{MoO}_3 \leftrightarrow \text{P}$                                  | 0.017225 |
| 18.935                               | $\text{P}_2\text{O}_5 \cdot 24\text{MoO}_3 \leftrightarrow \text{PO}_4$                               | 0.052813 |
| 25.338                               | $\text{P}_2\text{O}_5 \cdot 24\text{MoO}_3 \leftrightarrow \text{P}_2\text{O}_5$                      | 0.039466 |
| 11.526                               | $\text{U}_2\text{P}_2\text{O}_{11} \leftrightarrow \text{P}$                                          | 0.086762 |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                        |                                                                                             | Factor  |
|-------------------------------|---------------------------------------------------------------------------------------------|---------|
| <b>PHOSPHORUS (continued)</b> |                                                                                             |         |
| <b>P = 30.9738</b>            |                                                                                             |         |
| 3.7590                        | $\text{U}_2\text{P}_2\text{O}_{11} \leftrightarrow \text{PO}_4$                             | 0.26603 |
| 5.0303                        | $\text{U}_2\text{P}_2\text{O}_{11} \leftrightarrow \text{P}_2\text{O}_5$                    | 0.19880 |
| <b>PLATINUM</b>               |                                                                                             |         |
| <b>Pt = 195.09</b>            |                                                                                             |         |
| 0.93839                       | $\text{K}_2\text{PtCl}_6 \leftrightarrow \text{H}_2\text{PtCl}_6 \cdot 6\text{H}_2\text{O}$ | 1.0657  |
| 2.4912                        | $\text{K}_2\text{PtCl}_6 \leftrightarrow \text{Pt}$                                         | 0.40141 |
| 1.4426                        | $\text{K}_2\text{PtCl}_6 \leftrightarrow \text{PtCl}_4$                                     | 0.69320 |
| 1.1383                        | $\text{K}_2\text{PtCl}_6 \leftrightarrow \text{PtCl}_4 \cdot 5\text{H}_2\text{O}$           | 0.87854 |
| 2.2753                        | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{Pt}$                                    | 0.43950 |
| 1.3176                        | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{PtCl}_4$                                | 0.75897 |
| 1.0885                        | $(\text{NH}_4)_2\text{PtCl}_6 \leftrightarrow \text{PtCl}_6$                                | 0.91872 |
| 0.37668                       | $\text{Pt} \leftrightarrow \text{H}_2\text{PtCl}_6 \cdot 6\text{H}_2\text{O}$               | 2.6548  |
| 0.57907                       | $\text{Pt} \leftrightarrow \text{PtCl}_4$                                                   | 1.7269  |
| 0.45691                       | $\text{Pt} \leftrightarrow \text{PtCl}_4 \cdot 5\text{H}_2\text{O}$                         | 2.1886  |
| <b>POTASSIUM</b>              |                                                                                             |         |
| <b>K = 39.098</b>             |                                                                                             |         |
| 0.90639                       | $\text{Ag} \leftrightarrow \text{KBr}$                                                      | 1.1033  |
| 1.4469                        | $\text{Ag} \leftrightarrow \text{KCl}$                                                      | 0.69116 |
| 0.88021                       | $\text{Ag} \leftrightarrow \text{KClO}_3$                                                   | 1.1361  |
| 0.77856                       | $\text{Ag} \leftrightarrow \text{KClO}_4$                                                   | 1.2844  |
| 1.6565                        | $\text{Ag} \leftrightarrow \text{KCN}$                                                      | 0.60369 |
| 0.64978                       | $\text{Ag} \leftrightarrow \text{KI}$                                                       | 1.5390  |
| 1.5779                        | $\text{AgBr} \leftrightarrow \text{KBr}$                                                    | 0.63377 |
| 1.1244                        | $\text{AgBr} \leftrightarrow \text{KBrO}_3$                                                 | 0.88939 |
| 1.9223                        | $\text{AgCl} \leftrightarrow \text{KCl}$                                                    | 0.52020 |
| 1.1695                        | $\text{AgCl} \leftrightarrow \text{KClO}_3$                                                 | 0.85508 |
| 1.0344                        | $\text{AgCl} \leftrightarrow \text{KClO}_4$                                                 | 0.96672 |
| 2.0561                        | $\text{AgCN} \leftrightarrow \text{KCN}$                                                    | 0.48637 |
| 1.4142                        | $\text{AgI} \leftrightarrow \text{KI}$                                                      | 0.70712 |
| 1.0971                        | $\text{AgI} \leftrightarrow \text{KIO}_3$                                                   | 0.91153 |
| 1.3045                        | $\text{BaCrO}_4 \leftrightarrow \text{K}_2\text{CrO}_4$                                     | 0.76659 |
| 1.7222                        | $\text{BaCrO}_4 \leftrightarrow \text{K}_2\text{Cr}_2\text{O}_7$                            | 0.58065 |
| 1.7140                        | $\text{BaSO}_4 \leftrightarrow \text{KHSO}_4$                                               | 0.58342 |
| 2.1166                        | $\text{BaSO}_4 \leftrightarrow \text{K}_2\text{S}$                                          | 0.47245 |
| 1.3393                        | $\text{BaSO}_4 \leftrightarrow \text{K}_2\text{SO}_4$                                       | 0.74666 |
| 2.0436                        | $\text{Br} \leftrightarrow \text{K}$                                                        | 0.48933 |
| 0.67145                       | $\text{Br} \leftrightarrow \text{KBr}$                                                      | 1.4893  |
| 0.41473                       | $\text{CaF}_2 \leftrightarrow \text{KF} \cdot 2\text{H}_2\text{O}$                          | 2.4112  |
| 0.72315                       | $\text{CaSO}_4 \leftrightarrow \text{KF} \cdot 2\text{H}_2\text{O}$                         | 1.3828  |
| 0.90668                       | $\text{Cl} \leftrightarrow \text{K}$                                                        | 1.1029  |
| 0.47553                       | $\text{Cl} \leftrightarrow \text{KCl}$                                                      | 2.1029  |
| 0.28929                       | $\text{Cl} \leftrightarrow \text{KClO}_3$                                                   | 3.4567  |
| 0.25589                       | $\text{Cl} \leftrightarrow \text{KClO}_4$                                                   | 3.9080  |
| 0.75269                       | $\text{Cl} \leftrightarrow \text{K}_2\text{O}$                                              | 1.3286  |
| 0.46718                       | $\text{CO}_2 \leftrightarrow \text{K}_2\text{O}$                                            | 2.1405  |
| 0.31843                       | $\text{CO}_2 \leftrightarrow \text{K}_2\text{CO}_3$                                         | 3.1404  |
| 0.76441                       | $\text{I} \leftrightarrow \text{KI}$                                                        | 1.3082  |
| 0.59299                       | $\text{I} \leftrightarrow \text{KIO}_3$                                                     | 1.6864  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                                |                                                                     | Factor  |
|---------------------------------------|---------------------------------------------------------------------|---------|
| <b>POTASSIUM</b> ( <i>continued</i> ) |                                                                     |         |
| <b>K = 39.098</b>                     |                                                                     |         |
| 0.31907                               | $K \leftrightarrow KClO_3$                                          | 3.1341  |
| 0.83016                               | $K \leftrightarrow K_2O$                                            | 1.2046  |
| 0.38673                               | $K \leftrightarrow KNO_3$                                           | 2.5858  |
| 3.0436                                | $KBr \leftrightarrow K$                                             | 0.32856 |
| 2.5267                                | $KBr \leftrightarrow K_2O$                                          | 0.39578 |
| 1.9067                                | $KCl \leftrightarrow K$                                             | 0.52447 |
| 1.0789                                | $KCl \leftrightarrow K_2CO_3$                                       | 0.92690 |
| 0.50685                               | $KCl \leftrightarrow K_2Cr_2O_7$                                    | 1.9730  |
| 0.74466                               | $KCl \leftrightarrow KHCO_3$                                        | 1.3429  |
| 0.73737                               | $KCl \leftrightarrow KNO_3$                                         | 1.3562  |
| 1.5829                                | $KCl \leftrightarrow K_2O$                                          | 0.63177 |
| 0.85563                               | $KCl \leftrightarrow K_2SO_4$                                       | 1.1687  |
| 1.6437                                | $KClO_3 \leftrightarrow KCl$                                        | 0.60836 |
| 3.5433                                | $KClO_4 \leftrightarrow K$                                          | 0.28222 |
| 1.8584                                | $KClO_4 \leftrightarrow KCl$                                        | 0.53811 |
| 2.9415                                | $KClO_4 \leftrightarrow K_2O$                                       | 0.33996 |
| 4.2456                                | $KI \leftrightarrow K$                                              | 0.23554 |
| 3.5245                                | $KI \leftrightarrow K_2O$                                           | 0.28373 |
| 0.38435                               | $K_2O \leftrightarrow KClO_3$                                       | 2.6018  |
| 0.68159                               | $K_2O \leftrightarrow K_2CO_3$                                      | 1.4672  |
| 0.32021                               | $K_2O \leftrightarrow K_2Cr_2O_7$                                   | 3.1229  |
| 0.47045                               | $K_2O \leftrightarrow KHCO_3$                                       | 2.1256  |
| 0.46584                               | $K_2O \leftrightarrow KNO_3$                                        | 2.1466  |
| 0.81194                               | $KOH \leftrightarrow K_2CO_3$                                       | 1.2316  |
| 1.1912                                | $KOH \leftrightarrow K_2O$                                          | 0.83946 |
| 6.2146                                | $K_2PtCl_6 \leftrightarrow K$                                       | 0.16091 |
| 3.5165                                | $K_2PtCl_6 \leftrightarrow K_2CO_3$                                 | 0.28438 |
| 3.2594                                | $K_2PtCl_6 \leftrightarrow KCl$                                     | 0.30680 |
| 2.4271                                | $K_2PtCl_6 \leftrightarrow KHCO_3$                                  | 0.41201 |
| 2.4034                                | $K_2PtCl_6 \leftrightarrow KNO_3$                                   | 0.41608 |
| 5.1592                                | $K_2PtCl_6 \leftrightarrow K_2O$                                    | 0.19383 |
| 2.7888                                | $K_2PtCl_6 \leftrightarrow K_2SO_4$                                 | 0.35857 |
| 0.51224                               | $K_2PtCl_6 \leftrightarrow K_2SO_4 \cdot Al_2(SO_4)_3 \cdot 24H_2O$ | 1.9522  |
| 0.48659                               | $K_2PtCl_6 \leftrightarrow K_2SO_4 \cdot Cr_2(SO_4)_3 \cdot 24H_2O$ | 2.0551  |
| 1.2609                                | $K_2SO_4 \leftrightarrow K_2CO_3$                                   | 0.79308 |
| 0.87031                               | $K_2SO_4 \leftrightarrow KHCO_3$                                    | 1.1490  |
| 0.63990                               | $K_2SO_4 \leftrightarrow KHSO_4$                                    | 1.5627  |
| 1.0238                                | $K_2SO_4 \leftrightarrow KNO_2$                                     | 0.97674 |
| 0.86179                               | $K_2SO_4 \leftrightarrow KNO_3$                                     | 1.1604  |
| 2.2285                                | $K_2SO_4 \leftrightarrow K$                                         | 0.44875 |
| 1.8499                                | $K_2SO_4 \leftrightarrow K_2O$                                      | 0.54056 |
| 1.5804                                | $K_2SO_4 \leftrightarrow K_2S$                                      | 0.63275 |
| 0.60582                               | $Mg_2As_2O_7 \leftrightarrow K_3AsO_4$                              | 1.6506  |
| 0.71164                               | $Mg_2As_2O_7 \leftrightarrow K_2HAsO_4$                             | 1.4052  |
| 0.40040                               | $Mn_2O_3 \leftrightarrow K_2MnO_4$                                  | 2.4975  |
| 0.49946                               | $Mn_2O_3 \leftrightarrow KMnO_4$                                    | 2.0022  |
| 0.44132                               | $MnS \leftrightarrow K_2MnO_4$                                      | 2.2659  |
| 0.55051                               | $MnS \leftrightarrow KMnO_4$                                        | 1.8165  |
| 0.13853                               | $N \leftrightarrow KNO_3$                                           | 7.2185  |
| 0.16844                               | $NH_3 \leftrightarrow KNO_3$                                        | 5.9368  |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                       |                                                                   | Factor  |
|------------------------------|-------------------------------------------------------------------|---------|
| <b>POTASSIUM (continued)</b> |                                                                   |         |
| <b>K = 39.098</b>            |                                                                   |         |
| 0.29677                      | $\text{NO} \leftrightarrow \text{KNO}_3$                          | 3.3697  |
| 0.44656                      | $\text{N}_2\text{O}_3 \leftrightarrow \text{KNO}_2$               | 2.2393  |
| 1.1466                       | $\text{N}_2\text{O}_5 \leftrightarrow \text{K}_2\text{O}$         | 0.87217 |
| 0.53412                      | $\text{N}_2\text{O}_5 \leftrightarrow \text{KNO}_3$               | 1.8722  |
| 2.4946                       | $\text{Pt} \leftrightarrow \text{K}$                              | 0.40086 |
| 1.3084                       | $\text{Pt} \leftrightarrow \text{KCl}$                            | 0.76431 |
| 2.0710                       | $\text{Pt} \leftrightarrow \text{K}_2\text{O}$                    | 0.48287 |
| 0.38943                      | $\text{SiO}_2 \leftrightarrow \text{K}_2\text{SiO}_3$             | 2.5679  |
| 0.45941                      | $\text{SO}_3 \leftrightarrow \text{K}_2\text{SO}_4$               | 2.1767  |
| <b>PRASEODYMIUM</b>          |                                                                   |         |
| <b>Pr = 140.908</b>          |                                                                   |         |
| 1.1703                       | $\text{Pr}_2\text{O}_3 \leftrightarrow \text{Pr}$                 | 0.85449 |
| <b>RHODIUM</b>               |                                                                   |         |
| <b>Rh = 102.905</b>          |                                                                   |         |
| 0.26758                      | $\text{Rh} \leftrightarrow \text{Na}_3\text{RhCl}_6$              | 3.7372  |
| 0.49178                      | $\text{Rh} \leftrightarrow \text{RhCl}_3$                         | 2.0334  |
| <b>RUBIDIUM</b>              |                                                                   |         |
| <b>Rb = 85.468</b>           |                                                                   |         |
| 1.6768                       | $\text{AgCl} \leftrightarrow \text{Rb}$                           | 0.59636 |
| 1.1852                       | $\text{AgCl} \leftrightarrow \text{RbCl}$                         | 0.84371 |
| 0.41480                      | $\text{Cl} \leftrightarrow \text{Rb}$                             | 2.4108  |
| 0.29319                      | $\text{Cl} \leftrightarrow \text{RbCl}$                           | 3.4107  |
| 0.70683                      | $\text{Rb} \leftrightarrow \text{RbCl}$                           | 1.4148  |
| 0.74016                      | $\text{Rb} \leftrightarrow \text{Rb}_2\text{CO}_3$                | 1.3511  |
| 0.91441                      | $\text{Rb} \leftrightarrow \text{Rb}_2\text{O}$                   | 1.0936  |
| 0.64023                      | $\text{Rb} \leftrightarrow \text{Rb}_2\text{SO}_4$                | 1.5620  |
| 1.0472                       | $\text{RbCl} \leftrightarrow \text{Rb}_2\text{CO}_3$              | 0.95497 |
| 0.90577                      | $\text{RbCl} \leftrightarrow \text{Rb}_2\text{SO}_4$              | 1.1040  |
| 2.1636                       | $\text{RbClO}_4 \leftrightarrow \text{Rb}$                        | 0.46220 |
| 0.78828                      | $\text{Rb}_2\text{CO}_3 \leftrightarrow \text{RbHCO}_3$           | 1.2686  |
| 0.77299                      | $\text{Rb}_2\text{O} \leftrightarrow \text{RbCl}$                 | 1.2937  |
| 0.70015                      | $\text{Rb}_2\text{O} \leftrightarrow \text{Rb}_2\text{SO}_4$      | 1.4283  |
| 3.3857                       | $\text{Rb}_2\text{PtCl}_6 \leftrightarrow \text{Rb}$              | 0.29536 |
| 2.3931                       | $\text{Rb}_2\text{PtCl}_6 \leftrightarrow \text{RbCl}$            | 0.41787 |
| 2.5060                       | $\text{Rb}_2\text{PtCl}_6 \leftrightarrow \text{Rb}_2\text{CO}_3$ | 0.39905 |
| 1.9754                       | $\text{Rb}_2\text{PtCl}_6 \leftrightarrow \text{RbHCO}_3$         | 0.50623 |
| 3.0959                       | $\text{Rb}_2\text{PtCl}_6 \leftrightarrow \text{Rb}_2\text{O}$    | 0.32301 |
| 1.1561                       | $\text{Rb}_2\text{SO}_4 \leftrightarrow \text{Rb}_2\text{CO}_3$   | 0.86498 |
| 0.91133                      | $\text{Rb}_2\text{SO}_4 \leftrightarrow \text{RbHCO}_3$           | 1.0973  |
| <b>SELENIUM</b>              |                                                                   |         |
| <b>Se = 78.96</b>            |                                                                   |         |
| 0.61224                      | $\text{Se} \leftrightarrow \text{H}_2\text{SeO}_3$                | 1.6334  |
| 0.54466                      | $\text{Se} \leftrightarrow \text{H}_2\text{SeO}_4$                | 1.8360  |
| 0.71161                      | $\text{Se} \leftrightarrow \text{SeO}_2$                          | 1.4053  |
| 0.62193                      | $\text{Se} \leftrightarrow \text{SeO}_3$                          | 1.6079  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor              |                                                                                   | Factor  |
|---------------------|-----------------------------------------------------------------------------------|---------|
| <b>SILICON</b>      |                                                                                   |         |
| <b>Si = 28.086</b>  |                                                                                   |         |
| 2.6847              | $\text{BaSiF}_6 \leftrightarrow \text{SiF}_4$                                     | 0.37249 |
| 4.6504              | $\text{BaSiF}_6 \leftrightarrow \text{SiO}_2$                                     | 0.21503 |
| 2.1163              | $\text{K}_2\text{SiF}_6 \leftrightarrow \text{SiF}_4$                             | 0.47249 |
| 3.6661              | $\text{K}_2\text{SiF}_6 \leftrightarrow \text{SiO}_2$                             | 0.27277 |
| 3.3384              | $\text{SiC} \leftrightarrow \text{C}$                                             | 0.29954 |
| 0.91111             | $\text{SiC} \leftrightarrow \text{CO}_2$                                          | 1.0976  |
| 0.76933             | $\text{SiO}_2 \leftrightarrow \text{H}_2\text{SiO}_3$                             | 1.2998  |
| 2.1393              | $\text{SiO}_2 \leftrightarrow \text{Si}$                                          | 0.46744 |
| 0.57730             | $\text{SiO}_2 \leftrightarrow \text{SiF}_4$                                       | 1.7322  |
| 0.78972             | $\text{SiO}_2 \leftrightarrow \text{SiO}_3$                                       | 1.2663  |
| 0.65250             | $\text{SiO}_2 \leftrightarrow \text{SiO}_4$                                       | 1.5326  |
| 1.6651              | $\text{SiO}_2 \leftrightarrow \text{Si}_2\text{O}$                                | 0.60057 |
| 0.62514             | $\text{SiO}_2 \leftrightarrow \text{Si}(\text{OH})_4$                             | 1.5997  |
| <b>SILVER</b>       |                                                                                   |         |
| <b>Ag = 107.868</b> |                                                                                   |         |
| 0.63501             | $\text{Ag} \leftrightarrow \text{AgNO}_3$                                         | 1.5748  |
| 0.93096             | $\text{Ag} \leftrightarrow \text{Ag}_2\text{O}$                                   | 1.0742  |
| 1.7408              | $\text{AgBr} \leftrightarrow \text{Ag}$                                           | 0.57445 |
| 1.3286              | $\text{AgCl} \leftrightarrow \text{Ag}$                                           | 0.75265 |
| 0.84371             | $\text{AgCl} \leftrightarrow \text{AgNO}_3$                                       | 1.1852  |
| 1.2369              | $\text{AgCl} \leftrightarrow \text{Ag}_2\text{O}$                                 | 0.80847 |
| 1.7935              | $\text{AgCl} \leftrightarrow \text{Br}$                                           | 0.55756 |
| 1.2412              | $\text{AgCN} \leftrightarrow \text{Ag}$                                           | 0.80566 |
| 2.1764              | $\text{AgI} \leftrightarrow \text{Ag}$                                            | 0.45947 |
| 1.2935              | $\text{Ag}_3\text{PO}_4 \leftrightarrow \text{Ag}$                                | 0.77311 |
| 1.4031              | $\text{Ag}_4\text{P}_2\text{O}_7 \leftrightarrow \text{Ag}$                       | 0.71269 |
| 0.74079             | $\text{Br} \leftrightarrow \text{Ag}$                                             | 1.3499  |
| 0.42555             | $\text{Br} \leftrightarrow \text{AgBr}$                                           | 2.3499  |
| 0.32866             | $\text{Cl} \leftrightarrow \text{Ag}$                                             | 3.0426  |
| 0.24737             | $\text{Cl} \leftrightarrow \text{AgCl}$                                           | 4.0425  |
| 1.1764              | $\text{I} \leftrightarrow \text{Ag}$                                              | 0.85004 |
| 0.54053             | $\text{I} \leftrightarrow \text{AgI}$                                             | 1.8500  |
| <b>SODIUM</b>       |                                                                                   |         |
| <b>Na = 22.9898</b> |                                                                                   |         |
| 1.0483              | $\text{Ag} \leftrightarrow \text{NaBr}$                                           | 0.95393 |
| 1.8457              | $\text{Ag} \leftrightarrow \text{NaCl}$                                           | 0.54179 |
| 0.71966             | $\text{Ag} \leftrightarrow \text{NaI}$                                            | 1.3895  |
| 1.8249              | $\text{AgBr} \leftrightarrow \text{NaBr}$                                         | 0.54798 |
| 2.4523              | $\text{AgCl} \leftrightarrow \text{NaCl}$                                         | 0.40778 |
| 1.5663              | $\text{AgI} \leftrightarrow \text{NaI}$                                           | 0.63845 |
| 1.9440              | $\text{BaSO}_4 \leftrightarrow \text{NaHSO}_4$                                    | 0.51440 |
| 1.6905              | $\text{BaSO}_4 \leftrightarrow \text{NaHSO}_4 \cdot \text{H}_2\text{O}$           | 0.59156 |
| 2.9906              | $\text{BaSO}_4 \leftrightarrow \text{Na}_2\text{S}$                               | 0.33438 |
| 1.8518              | $\text{BaSO}_4 \leftrightarrow \text{Na}_2\text{SO}_3$                            | 0.54002 |
| 0.92564             | $\text{BaSO}_4 \leftrightarrow \text{Na}_2\text{SO}_3 \cdot 7\text{H}_2\text{O}$  | 1.0803  |
| 1.6432              | $\text{BaSO}_4 \leftrightarrow \text{Na}_2\text{SO}_4$                            | 0.60857 |
| 0.72442             | $\text{BaSO}_4 \leftrightarrow \text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$ | 1.3804  |



TABLE 11.19 Gravimetric Factors (Continued)

| Factor                    |                                                                                     | Factor   |
|---------------------------|-------------------------------------------------------------------------------------|----------|
| <b>SODIUM (continued)</b> |                                                                                     |          |
| <b>Na = 22.9898</b>       |                                                                                     |          |
| 0.69198                   | $B_2O_3 \leftrightarrow Na_2B_4O_7$                                                 | 1.4451   |
| 0.36510                   | $B_2O_3 \leftrightarrow Na_2B_4O_7 \cdot 10H_2O$                                    | 2.7389   |
| 3.4758                    | $Br \leftrightarrow Na$                                                             | 0.28770  |
| 0.77657                   | $Br \leftrightarrow NaBr$                                                           | 1.2877   |
| 2.5786                    | $Br \leftrightarrow Na_2O$                                                          | 0.38781  |
| 0.94956                   | $CaCl_2 \leftrightarrow NaCl$                                                       | 1.0531   |
| 0.94433                   | $CaCO_3 \leftrightarrow Na_2CO_3$                                                   | 1.0590   |
| 0.92975                   | $CaF_2 \leftrightarrow NaF$                                                         | 1.0756   |
| 0.52910                   | $CaO \leftrightarrow Na_2CO_3$                                                      | 1.8900   |
| 1.2845                    | $CaSO_4 \leftrightarrow Na_2CO_3$                                                   | 0.77854  |
| 1.5421                    | $Cl \leftrightarrow Na$                                                             | 0.64846  |
| 0.60663                   | $Cl \leftrightarrow NaCl$                                                           | 1.6485   |
| 1.1442                    | $Cl \leftrightarrow Na_2O$                                                          | 0.87410  |
| 0.41520                   | $CO_2 \leftrightarrow Na_2CO_3$                                                     | 2.4083   |
| 0.71008                   | $CO_2 \leftrightarrow Na_2O$                                                        | 1.4083   |
| 1.2292                    | $H_3BO_3 \leftrightarrow Na_2B_4O_7$                                                | 0.81357  |
| 0.64853                   | $H_3BO_3 \leftrightarrow Na_2B_4O_7 \cdot 10H_2O$                                   | 1.5419   |
| 5.5198                    | $I \leftrightarrow Na$                                                              | 0.18117  |
| 0.84662                   | $I \leftrightarrow NaI$                                                             | 1.1812   |
| 4.0949                    | $I \leftrightarrow Na_2O$                                                           | 0.24420  |
| 2.5029                    | $KBF_4 \leftrightarrow Na_2B_4O_7$                                                  | 0.39954  |
| 1.3206                    | $KBF_4 \leftrightarrow Na_2B_4O_7 \cdot 10H_2O$                                     | 0.75724  |
| 0.91360                   | $Mg_2As_2O_7 \leftrightarrow Na_2HAsO_3$                                            | 1.0946   |
| 0.83497                   | $Mg_2As_2O_7 \leftrightarrow Na_2HAsO_4$                                            | 1.1976   |
| 0.81462                   | $MgCl_2 \leftrightarrow NaCl$                                                       | 1.2276   |
| 0.67882                   | $Mg_2P_2O_7 \leftrightarrow Na_3PO_4$                                               | 1.4731   |
| 0.78392                   | $Mg_2P_2O_7 \leftrightarrow Na_2HPO_4$                                              | 1.2757   |
| 0.31073                   | $Mg_2P_2O_7 \leftrightarrow NaHPO_4 \cdot 12H_2O$                                   | 3.2182   |
| 0.53229                   | $Mg_2P_2O_7 \leftrightarrow NaNH_4 \cdot HPO_4 \cdot 4H_2O$                         | 1.8787   |
| 0.49897                   | $Mg_2P_2O_7 \leftrightarrow Na_4P_2O_7 \cdot 10H_2O$                                | 2.0041   |
| 4.4759                    | $NaBr \leftrightarrow Na$                                                           | 0.22342  |
| 3.3205                    | $NaBr \leftrightarrow Na_2O$                                                        | 0.30116  |
| 65.502                    | $NaOAc \cdot Mg(OAc)_2 \cdot UO_2(OAc)_2 \cdot 6\frac{1}{2}H_2O \leftrightarrow Na$ | 0.015267 |
| 14.635                    | Triple $MgOAc \leftrightarrow NaBr$                                                 | 0.066331 |
| 28.416                    | Triple $MgOAc \leftrightarrow Na_2CO_3$                                             | 0.035192 |
| 25.768                    | Triple $MgOAc \leftrightarrow NaCl$                                                 | 0.038809 |
| 17.926                    | Triple $MgOAc \leftrightarrow NaHCO_3$                                              | 0.055785 |
| 10.047                    | Triple $MgOAc \leftrightarrow NaI$                                                  | 0.099535 |
| 37.650                    | Triple $MgOAc \leftrightarrow NaOH$                                                 | 0.026560 |
| 48.594                    | Triple $MgOAc \leftrightarrow Na_2O$                                                | 0.020579 |
| 21.204                    | Triple $MgOAc \leftrightarrow Na_2SO_4$                                             | 0.047161 |
| 66.894                    | $NaOAc \cdot Zn(OAc)_2 \cdot UO_3(OAc)_2 \cdot 6H_2O \leftrightarrow Na$            | 0.014949 |
| 14.946                    | Triple $ZnOAc \leftrightarrow NaBr$                                                 | 0.066909 |
| 29.020                    | Triple $ZnOAc \leftrightarrow Na_2CO_3$                                             | 0.034459 |
| 26.315                    | Triple $ZnOAc \leftrightarrow NaCl$                                                 | 0.038002 |
| 18.307                    | Triple $ZnOAc \leftrightarrow NaHCO_3$                                              | 0.054624 |
| 10.260                    | Triple $ZnOAc \leftrightarrow NaI$                                                  | 0.097464 |
| 38.451                    | Triple $ZnOAc \leftrightarrow NaOH$                                                 | 0.026008 |
| 49.626                    | Triple $ZnOAc \leftrightarrow Na_2O$                                                | 0.020151 |
| 21.654                    | Triple $ZnOAc \leftrightarrow Na_2SO_4$                                             | 0.046180 |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor                             |                                                                                                      | Factor  |
|------------------------------------|------------------------------------------------------------------------------------------------------|---------|
| <b>SODIUM</b> ( <i>continued</i> ) |                                                                                                      |         |
| <b>Na = 22.9898</b>                |                                                                                                      |         |
| 2.5421                             | $\text{NaCl} \leftrightarrow \text{Na}$                                                              | 0.39337 |
| 1.1028                             | $\text{NaCl} \leftrightarrow \text{Na}_2\text{CO}_3$                                                 | 0.90678 |
| 0.69569                            | $\text{NaCl} \leftrightarrow \text{NaHCO}_3$                                                         | 1.4374  |
| 0.82337                            | $\text{NaCl} \leftrightarrow \text{Na}_2\text{HPO}_4$                                                | 1.2145  |
| 1.8859                             | $\text{NaCl} \leftrightarrow \text{Na}_2\text{O}$                                                    | 0.53025 |
| 0.82291                            | $\text{NaCl} \leftrightarrow \text{Na}_2\text{SO}_4$                                                 | 1.2152  |
| 0.74267                            | $\text{NaClO}_3 \leftrightarrow \text{AgCl}$                                                         | 1.3465  |
| 1.8213                             | $\text{NaClO}_3 \leftrightarrow \text{NaCl}$                                                         | 0.54907 |
| 0.85432                            | $\text{NaClO}_4 \leftrightarrow \text{AgCl}$                                                         | 1.1705  |
| 2.0950                             | $\text{NaClO}_4 \leftrightarrow \text{NaCl}$                                                         | 0.47732 |
| 2.3051                             | $\text{Na}_2\text{CO}_3 \leftrightarrow \text{Na}$                                                   | 0.43381 |
| 0.63084                            | $\text{Na}_2\text{CO}_3 \leftrightarrow \text{NaHCO}_3$                                              | 1.5852  |
| 1.7101                             | $\text{Na}_2\text{CO}_3 \leftrightarrow \text{Na}_2\text{O}$                                         | 0.58476 |
| 1.3250                             | $\text{Na}_2\text{CO}_3 \leftrightarrow \text{NaOH}$                                                 | 0.75473 |
| 3.6541                             | $\text{NaHCO}_3 \leftrightarrow \text{Na}$                                                           | 0.27367 |
| 2.7108                             | $\text{NaHCO}_3 \leftrightarrow \text{Na}_2\text{O}$                                                 | 0.36889 |
| 6.5198                             | $\text{NaI} \leftrightarrow \text{Na}$                                                               | 0.15338 |
| 4.8368                             | $\text{NaI} \leftrightarrow \text{Na}_2\text{O}$                                                     | 0.20675 |
| 1.3480                             | $\text{Na}_2\text{O} \leftrightarrow \text{Na}$                                                      | 0.74186 |
| 0.43659                            | $\text{Na}_2\text{O} \leftrightarrow \text{Na}_2\text{HPO}_4$                                        | 2.2905  |
| 0.36460                            | $\text{Na}_2\text{O} \leftrightarrow \text{NaNO}_3$                                                  | 2.7427  |
| 0.77480                            | $\text{Na}_2\text{O} \leftrightarrow \text{NaOH}$                                                    | 1.2907  |
| 0.93653                            | $\text{Na}_4\text{P}_2\text{O}_7 \leftrightarrow \text{Na}_2\text{HPO}_4$                            | 1.0678  |
| 0.37122                            | $\text{Na}_4\text{P}_2\text{O}_7 \leftrightarrow \text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$ | 2.6938  |
| 3.0892                             | $\text{Na}_2\text{SO}_4 \leftrightarrow \text{Na}$                                                   | 0.32371 |
| 1.3401                             | $\text{Na}_2\text{SO}_4 \leftrightarrow \text{Na}_2\text{CO}_3$                                      | 0.74620 |
| 0.49640                            | $\text{Na}_2\text{SO}_4 \leftrightarrow \text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$           | 2.0145  |
| 2.2917                             | $\text{Na}_2\text{SO}_4 \leftrightarrow \text{Na}_2\text{O}$                                         | 0.43635 |
| 0.16480                            | $\text{N} \leftrightarrow \text{NaNO}_3$                                                             | 6.0680  |
| 0.20038                            | $\text{NH}_3 \leftrightarrow \text{NaNO}_3$                                                          | 4.9906  |
| 0.081461                           | $\text{NH}_3 \leftrightarrow \text{NaNH}_4\text{HPO}_4 \cdot 4\text{H}_2\text{O}$                    | 12.276  |
| 0.35303                            | $\text{NO} \leftrightarrow \text{NaNO}_3$                                                            | 2.8326  |
| 0.63539                            | $\text{N}_2\text{O}_5 \leftrightarrow \text{NaNO}_3$                                                 | 1.5738  |
| 1.7427                             | $\text{N}_2\text{O}_5 \leftrightarrow \text{Na}_2\text{O}$                                           | 0.57383 |
| 0.49993                            | $\text{P}_2\text{O}_5 \leftrightarrow \text{Na}_2\text{HPO}_4$                                       | 2.0003  |
| 0.19816                            | $\text{P}_2\text{O}_5 \leftrightarrow \text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$            | 5.0464  |
| 0.33946                            | $\text{P}_2\text{O}_5 \leftrightarrow \text{NaNH}_4\text{HPO}_4 \cdot \text{H}_2\text{O}$            | 2.9459  |
| 0.61564                            | $\text{SO}_2 \leftrightarrow \text{NaHSO}_3$                                                         | 1.6243  |
| 0.50828                            | $\text{SO}_2 \leftrightarrow \text{Na}_2\text{SO}_3$                                                 | 1.9674  |
| 0.25407                            | $\text{SO}_2 \leftrightarrow \text{Na}_2\text{SO}_3 \cdot 7\text{H}_2\text{O}$                       | 3.9360  |
| 1.2918                             | $\text{SO}_2 \leftrightarrow \text{Na}_2\text{O}$                                                    | 0.77414 |
| 0.56366                            | $\text{SO}_2 \leftrightarrow \text{Na}_2\text{SO}_4$                                                 | 1.7741  |
| <b>STRONTIUM</b>                   |                                                                                                      |         |
| <b>Sr = 87.62</b>                  |                                                                                                      |         |
| 0.29811                            | $\text{CO}_2 \leftrightarrow \text{SrCO}_3$                                                          | 3.3545  |
| 0.77265                            | $\text{SO}_3 \leftrightarrow \text{SrO}$                                                             | 1.2942  |
| 0.43588                            | $\text{SO}_3 \leftrightarrow \text{SrSO}_4$                                                          | 2.2942  |
| 0.41402                            | $\text{Sr} \leftrightarrow \text{Sr}(\text{NO}_3)_2$                                                 | 2.4153  |
| 1.6849                             | $\text{SrCO}_3 \leftrightarrow \text{Sr}$                                                            | 0.59351 |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor                       |                                                                              | Factor   |
|------------------------------|------------------------------------------------------------------------------|----------|
| <b>STRONTIUM</b> (continued) |                                                                              |          |
| <b>Sr = 87.62</b>            |                                                                              |          |
| 0.93124                      | $\text{SrCO}_3 \leftrightarrow \text{SrCl}_2$                                | 1.0738   |
| 0.70424                      | $\text{SrCO}_3 \leftrightarrow \text{Sr}(\text{HCO}_3)_2$                    | 1.4200   |
| 0.69759                      | $\text{SrCO}_3 \leftrightarrow \text{Sr}(\text{NO}_3)_2$                     | 1.4335   |
| 1.1826                       | $\text{SrO} \leftrightarrow \text{Sr}$                                       | 0.84559  |
| 0.65363                      | $\text{SrO} \leftrightarrow \text{SrCl}_2$                                   | 1.5299   |
| 0.70189                      | $\text{SrO} \leftrightarrow \text{SrCO}_3$                                   | 1.4247   |
| 0.49430                      | $\text{SrO} \leftrightarrow \text{Sr}(\text{HCO}_3)_2$                       | 2.0231   |
| 0.48963                      | $\text{SrO} \leftrightarrow \text{Sr}(\text{NO}_3)_2$                        | 2.0424   |
| 2.0963                       | $\text{SrSO}_4 \leftrightarrow \text{Sr}$                                    | 0.47703  |
| 1.1586                       | $\text{SrSO}_4 \leftrightarrow \text{SrCl}_2$                                | 0.86308  |
| 1.2442                       | $\text{SrSO}_4 \leftrightarrow \text{SrCO}_3$                                | 0.80373  |
| 0.86793                      | $\text{SrSO}_4 \leftrightarrow \text{Sr}(\text{NO}_3)_2$                     | 1.1522   |
| 1.7726                       | $\text{SrSO}_4 \leftrightarrow \text{SrO}$                                   | 0.56413  |
| <b>SULFUR</b>                |                                                                              |          |
| <b>S = 32.06</b>             |                                                                              |          |
| 2.4064                       | $\text{As}_2\text{S}_3 \leftrightarrow \text{H}_2\text{S}$                   | 0.41556  |
| 2.5577                       | $\text{As}_2\text{S}_3 \leftrightarrow \text{S}$                             | 0.39097  |
| 3.8906                       | $\text{BaSO}_4 \leftrightarrow \text{FeS}_2$                                 | 0.25703  |
| 6.8486                       | $\text{BaSO}_4 \leftrightarrow \text{H}_2\text{S}$                           | 0.14602  |
| 2.8436                       | $\text{BaSO}_4 \leftrightarrow \text{H}_2\text{SO}_3$                        | 0.35166  |
| 2.3797                       | $\text{BaSO}_4 \leftrightarrow \text{H}_2\text{SO}_4$                        | 0.42022  |
| 7.2792                       | $\text{BaSO}_4 \leftrightarrow \text{S}$                                     | 0.13738  |
| 3.6433                       | $\text{BaSO}_4 \leftrightarrow \text{SO}_2$                                  | 0.27448  |
| 2.9152                       | $\text{BaSO}_4 \leftrightarrow \text{SO}_3$                                  | 0.34302  |
| 2.4297                       | $\text{BaSO}_4 \leftrightarrow \text{SO}_4$                                  | 0.41158  |
| 4.2388                       | $\text{CdS} \leftrightarrow \text{H}_2\text{S}$                              | 0.23591  |
| 4.5054                       | $\text{CdS} \leftrightarrow \text{S}$                                        | 0.22196  |
| 1.2250                       | $\text{H}_2\text{SO}_4 \leftrightarrow \text{SO}_3$                          | 0.81631  |
| 1.6505                       | $(\text{NH}_4)_2\text{SO}_4 \leftrightarrow \text{SO}_3$                     | 0.60589  |
| 1.3473                       | $(\text{NH}_4)_2\text{SO}_4 \leftrightarrow \text{H}_2\text{SO}_4$           | 0.74223  |
| 2.3492                       | $\text{SO}_3 \leftrightarrow \text{H}_2\text{S}$                             | 0.42567  |
| <b>TANTALUM</b>              |                                                                              |          |
| <b>Ta = 180.948</b>          |                                                                              |          |
| 0.81898                      | $\text{Ta} \leftrightarrow \text{Ta}_2\text{O}_5$                            | 1.2210   |
| 0.50515                      | $\text{Ta} \leftrightarrow \text{TaCl}_5$                                    | 1.9796   |
| 16.065                       | $\text{TaC} \leftrightarrow \text{C}$                                        | 0.062246 |
| 1.0664                       | $\text{TaC} \leftrightarrow \text{Ta}$                                       | 0.93776  |
| 0.61680                      | $\text{Ta}_2\text{O}_5 \leftrightarrow \text{TaCl}_5$                        | 1.6213   |
| 1.0376                       | $\text{Ta}_2\text{O}_5 \leftrightarrow \text{Ta}_2\text{O}_4$                | 0.96379  |
| <b>TELLURIUM</b>             |                                                                              |          |
| <b>Te = 127.60</b>           |                                                                              |          |
| 0.65906                      | $\text{Te} \leftrightarrow \text{H}_2\text{TeO}_4$                           | 1.5173   |
| 0.55565                      | $\text{Te} \leftrightarrow \text{H}_2\text{TeO}_4 \cdot 2\text{H}_2\text{O}$ | 1.7997   |
| 0.79950                      | $\text{Te} \leftrightarrow \text{TeO}_2$                                     | 1.2508   |
| 0.72665                      | $\text{Te} \leftrightarrow \text{TeO}_3$                                     | 1.3762   |
| 1.5645                       | $(\text{TeO}_2)_2\text{SO}_3 \leftrightarrow \text{Te}$                      | 0.63918  |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor              |                                                                                   | Factor  |
|---------------------|-----------------------------------------------------------------------------------|---------|
| <b>THALLIUM</b>     |                                                                                   |         |
| <b>Tl = 204.37</b>  |                                                                                   |         |
| 0.87198             | $\text{Tl} \leftrightarrow \text{Tl}_2\text{CO}_3$                                | 1.1468  |
| 0.85218             | $\text{Tl} \leftrightarrow \text{TlCl}$                                           | 1.1735  |
| 0.61693             | $\text{Tl} \leftrightarrow \text{TlI}$                                            | 1.6209  |
| 0.76724             | $\text{Tl} \leftrightarrow \text{TlNO}_3$                                         | 1.3034  |
| 0.96232             | $\text{Tl} \leftrightarrow \text{Tl}_2\text{O}$                                   | 1.0391  |
| 1.2838              | $\text{Tl}_2\text{CrO}_4 \leftrightarrow \text{Tl}$                               | 0.77895 |
| 1.4750              | $\text{TiHSO}_4 \leftrightarrow \text{Tl}$                                        | 0.67798 |
| 1.9977              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{Tl}$                              | 0.50057 |
| 1.7024              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{TlCl}$                            | 0.58740 |
| 1.7420              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{Tl}_2\text{CO}_3$                 | 0.57406 |
| 1.2325              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{TlI}$                             | 0.81139 |
| 1.5327              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{TlNO}_3$                          | 0.65243 |
| 1.9225              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{Tl}_2\text{O}$                    | 0.52017 |
| 1.6176              | $\text{Tl}_2\text{PtCl}_6 \leftrightarrow \text{Tl}_2\text{SO}_4$                 | 0.61821 |
| 1.2350              | $\text{Tl}_2\text{SO}_4 \leftrightarrow \text{Tl}$                                | 0.80971 |
| <b>THORIUM</b>      |                                                                                   |         |
| <b>Th = 232.038</b> |                                                                                   |         |
| 1.1379              | $\text{ThO}_2 \leftrightarrow \text{Th}$                                          | 0.87881 |
| 0.70627             | $\text{ThO}_2 \leftrightarrow \text{ThCl}_4$                                      | 1.4159  |
| 0.44893             | $\text{ThO}_2 \leftrightarrow \text{Th}(\text{NO}_3)_4 \cdot 6\text{H}_2\text{O}$ | 2.2275  |
| <b>TIN</b>          |                                                                                   |         |
| <b>Sn = 118.69</b>  |                                                                                   |         |
| 0.62600             | $\text{Sn} \leftrightarrow \text{SnCl}_2$                                         | 1.5974  |
| 0.52604             | $\text{Sn} \leftrightarrow \text{SnCl}_2 \cdot 2\text{H}_2\text{O}$               | 1.9010  |
| 0.45562             | $\text{Sn} \leftrightarrow \text{SnCl}_4$                                         | 2.1948  |
| 0.32297             | $\text{Sn} \leftrightarrow \text{SnCl}_4 \cdot (\text{NH}_4\text{Cl})_2$          | 3.0962  |
| 0.88121             | $\text{Sn} \leftrightarrow \text{SnO}$                                            | 1.1348  |
| 0.78764             | $\text{Sn} \leftrightarrow \text{SnO}_2$                                          | 1.2696  |
| 0.79478             | $\text{SnO}_2 \leftrightarrow \text{SnCl}_2$                                      | 1.2582  |
| 0.66786             | $\text{SnO}_2 \leftrightarrow \text{SnCl}_2 \cdot 2\text{H}_2\text{O}$            | 1.4973  |
| 0.57846             | $\text{SnO}_2 \leftrightarrow \text{SnCl}_4$                                      | 1.7287  |
| 0.41005             | $\text{SnO}_2 \leftrightarrow \text{SnCl}_4 \cdot (\text{NH}_4\text{Cl})_2$       | 2.4387  |
| 1.1188              | $\text{SnO}_2 \leftrightarrow \text{SnO}$                                         | 0.89382 |
| <b>TITANIUM</b>     |                                                                                   |         |
| <b>Ti = 47.867</b>  |                                                                                   |         |
| 2.1059              | $\text{K}_2\text{TiF}_6 \leftrightarrow \text{F}$                                 | 0.47485 |
| 3.0699              | $\text{K}_2\text{TiF}_6 \leftrightarrow \text{K}$                                 | 0.32574 |
| 2.0660              | $\text{K}_2\text{TiF}_6 \leftrightarrow 2\text{KF}$                               | 0.48403 |
| 1.2752              | $\text{K}_2\text{TiF}_6 \leftrightarrow 2(\text{KF} \cdot 2\text{H}_2\text{O})$   | 0.78421 |
| 5.0150              | $\text{K}_2\text{TiF}_6 \leftrightarrow \text{Ti}$                                | 0.19940 |
| 3.0057              | $\text{K}_2\text{TiF}_6 \leftrightarrow \text{TiO}_2$                             | 0.33270 |
| 3.9853              | $\text{Ti} \leftrightarrow \text{C}$                                              | 0.25092 |
| 4.9853              | $\text{TiC} \leftrightarrow \text{C}$                                             | 0.20059 |
| 1.2509              | $\text{TiC} \leftrightarrow \text{Ti}$                                            | 0.79940 |
| 1.6299              | $\text{TiF}_4 \leftrightarrow \text{F}$                                           | 0.61354 |
| 1.6685              | $\text{TiO}_2 \leftrightarrow \text{Ti}$                                          | 0.59934 |

TABLE 11.19 Gravimetric Factors (Continued)

| Factor             |                                                                                             | Factor   |
|--------------------|---------------------------------------------------------------------------------------------|----------|
| <b>TUNGSTEN</b>    |                                                                                             |          |
| <b>W = 183.85</b>  |                                                                                             |          |
| 3.9348             | $\text{FeWO}_4 \leftrightarrow \text{Fe}_3\text{O}_4$                                       | 0.25414  |
| 1.3099             | $\text{FeWO}_4 \leftrightarrow \text{WO}_3$                                                 | 0.76344  |
| 6.7515             | $\text{MgWO}_4 \leftrightarrow \text{MgO}$                                                  | 0.14812  |
| 1.1739             | $\text{MgWO}_4 \leftrightarrow \text{WO}_3$                                                 | 0.85189  |
| 4.2684             | $\text{MnWO}_4 \leftrightarrow \text{MnO}$                                                  | 0.23428  |
| 1.3060             | $\text{MnWO}_4 \leftrightarrow \text{WO}_3$                                                 | 0.76571  |
| 2.0387             | $\text{PbWO}_4 \leftrightarrow \text{PbO}$                                                  | 0.49051  |
| 2.4751             | $\text{PbWO}_4 \leftrightarrow \text{W}$                                                    | 0.40403  |
| 1.9626             | $\text{PbWO}_4 \leftrightarrow \text{WO}_3$                                                 | 0.50952  |
| 15.307             | $\text{W} \leftrightarrow \text{C}$                                                         | 0.065330 |
| 0.96837            | $\text{W} \leftrightarrow \text{W}_2\text{C}$                                               | 1.0327   |
| 0.93868            | $\text{W} \leftrightarrow \text{WC}$                                                        | 1.0653   |
| 31.614             | $\text{W}_2\text{C} \leftrightarrow \text{C}$                                               | 0.031632 |
| 16.307             | $\text{WC} \leftrightarrow \text{C}$                                                        | 0.061324 |
| 1.1741             | $\text{WO}_2 \leftrightarrow \text{W}$                                                      | 0.85175  |
| 4.1515             | $\text{WO}_3 \leftrightarrow \text{Fe}$                                                     | 0.24088  |
| 1.2611             | $\text{WO}_3 \leftrightarrow \text{W}$                                                      | 0.79297  |
| <b>URANIUM</b>     |                                                                                             |          |
| <b>U = 238.03</b>  |                                                                                             |          |
| 1.1344             | $\text{UO}_2 \leftrightarrow \text{U}$                                                      | 0.88149  |
| 1.1792             | $\text{U}_3\text{O}_8 \leftrightarrow \text{U}$                                             | 0.84800  |
| 1.0395             | $\text{U}_3\text{O}_8 \leftrightarrow \text{UO}_2$                                          | 0.96200  |
| 0.55901            | $\text{U}_3\text{O}_8 \leftrightarrow \text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ | 1.7889   |
| 1.4998             | $\text{U}_2\text{P}_2\text{O}_{11} \leftrightarrow \text{U}$                                | 0.66675  |
| 1.3221             | $\text{U}_2\text{P}_2\text{O}_{11} \leftrightarrow \text{UO}_2$                             | 0.75639  |
| <b>VANADIUM</b>    |                                                                                             |          |
| <b>V = 50.941</b>  |                                                                                             |          |
| 5.2413             | $\text{VC} \leftrightarrow \text{C}$                                                        | 0.19079  |
| 1.7852             | $\text{V}_2\text{O}_5 \leftrightarrow \text{V}$                                             | 0.56017  |
| 0.79120            | $\text{V}_2\text{O}_5 \leftrightarrow \text{VO}_4$                                          | 1.2639   |
| <b>YTTERBIUM</b>   |                                                                                             |          |
| <b>Yb = 173.04</b> |                                                                                             |          |
| 1.1387             | $\text{Yb}_2\text{O}_3 \leftrightarrow \text{Yb}$                                           | 0.87820  |
| <b>ZINC</b>        |                                                                                             |          |
| <b>Zn = 65.38</b>  |                                                                                             |          |
| 2.3955             | $\text{BaSO}_4 \leftrightarrow \text{ZnS}$                                                  | 0.41745  |
| 0.81171            | $\text{BaSO}_4 \leftrightarrow \text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$                     | 1.2320   |
| 0.80338            | $\text{Zn} \leftrightarrow \text{ZnO}$                                                      | 1.2447   |
| 2.7288             | $\text{ZnNH}_4\text{PO}_4 \leftrightarrow \text{Zn}$                                        | 0.36646  |
| 2.1922             | $\text{ZnNH}_4\text{PO}_4 \leftrightarrow \text{ZnO}$                                       | 0.45616  |
| 0.59707            | $\text{ZnO} \leftrightarrow \text{ZnCl}_2$                                                  | 1.6748   |
| 0.64898            | $\text{ZnO} \leftrightarrow \text{ZnCO}_3$                                                  | 1.5409   |
| 0.28298            | $\text{ZnO} \leftrightarrow \text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$                        | 3.5338   |
| 2.3304             | $\text{Zn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{Zn}$                                 | 0.42911  |
| 1.8722             | $\text{Zn}_2\text{P}_2\text{O}_7 \leftrightarrow \text{ZnO}$                                | 0.53413  |
| 1.4905             | $\text{ZnS} \leftrightarrow \text{Zn}$                                                      | 0.67091  |
| 1.1974             | $\text{ZnS} \leftrightarrow \text{ZnO}$                                                     | 0.83512  |
| 0.33885            | $\text{ZnS} \leftrightarrow \text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$                        | 2.9511   |

**TABLE 11.19** Gravimetric Factors (*Continued*)

| Factor            |                                              | Factor  |
|-------------------|----------------------------------------------|---------|
| <b>ZIRCONIUM</b>  |                                              |         |
| <b>Zr = 91.22</b> |                                              |         |
| 2.4864            | $K_2ZrF_6 \leftrightarrow F$                 | 0.40219 |
| 2.4390            | $K_2ZrF_6 \leftrightarrow 2KF$               | 0.41001 |
| 1.5054            | $K_2ZrF_6 \leftrightarrow 2(KF \cdot 2H_2O)$ | 0.66427 |
| 3.1069            | $K_2ZrF_6 \leftrightarrow Zr$                | 0.32187 |
| 2.3000            | $K_2ZrF_6 \leftrightarrow ZrO_2$             | 0.43478 |
| 8.5946            | $ZrC \leftrightarrow C$                      | 0.11635 |
| 2.2004            | $ZrF_4 \leftrightarrow F$                    | 0.45447 |
| 1.3508            | $ZrO_2 \leftrightarrow Zr$                   | 0.74030 |
| 0.46470           | $ZrO_2 \leftrightarrow ZrP_2O_7$             | 2.1519  |

**TABLE 11.20** Elements Precipitated by General Analytical Reagents

This table includes the more common reagents used in gravimetric determinations. The lists of elements precipitated are not in all cases exhaustive. The usual solvent for a precipitating agent is indicated in parentheses after its name or formula. When the symbol of an element or radical is italicized, the element may be quantitatively determined by the use of the reagent in question.

| Reagent                                                               | Conditions                                                                                                                            | Substances precipitated                                                                                                    |
|-----------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| Ammonia, $NH_3$ (aqueous)                                             | After removal of acid sulfide group.                                                                                                  | <i>Al, Au, Be, Co, Cr, Cu, Fe, Ga, In, Ir, La, Nb, Ni, Os, P, Pb, rare earths, Sc, Si, Sn, Ta, Th, Ti, U, V, Y, Zn, Zr</i> |
| Ammonium polysulfide, $(NH_4)_2S_x$ (aqueous)                         | After removal of acid sulfide and $(NH_4)_2S$ groups.                                                                                 | Co, Mn, Ni, Si, Ti, V, W, Zn                                                                                               |
| Anthranilic acid, $NH_2C_6H_4COOH$ (aqueous)                          | 1% aqueous solution (pH 6); Cu separated from others at pH 2.9.                                                                       | Ag, <i>Cd, Co, Cu, Fe, Hg, Mn, Ni, Pb, Zn</i>                                                                              |
| $\alpha$ -Benzoin oxime, $C_6H_5CHOHC(=NOH)C_6H_5$ (1–2% alcohol)     | (a) Strongly acid medium.                                                                                                             | (a) <i>Cr(VI), Mo(VI), Nb, Pd(II), Ta(V), V(V), W(VI)</i>                                                                  |
| Benzidine, $H_2NC_6H_4C_6H_4NH_2$ (alcohol), 0.1M HCl                 | (b) Ammoniacal tartrate medium.                                                                                                       | (b) Above list                                                                                                             |
| <i>N</i> -Benzoylphenylhydroxylamine, $C_6H_5CO(C_6H_5)NOH$ (aqueous) | Similar to cupferron ( <i>q.v.</i> ). Cu, Fe(III), and Al complexes can be weighed as such; Ti compound must be ignited to the oxide. | <i>Cd, Fe(III), IO_3^-, PO_4^{3-}, SO_4^{2-}, W(VI)</i><br>See Cupferron                                                   |
| Cinchonine, $C_{19}H_{21}N_2OH$ , 6M HCl                              |                                                                                                                                       | Ir, Mo, Pt, W                                                                                                              |
| Cupferron, $C_6H_5N(NO)ONH_4$ (aqueous)                               | Group precipitant for several higher-charged metal ions from strongly acid solution. Precipitate ignited to metal oxide.              | <i>Al, Bi, Cu, Fe, Ga, La, Mo, Nb, Pd, rare earths, Sb, Sn, Ta, Th, Ti, Tl, U, V, W, Zr</i>                                |
| 1,2-Cyclohexanedionedioxime                                           | More water soluble than dimethylglyoxime; less subject to coprecipitation with metal chelate.                                         | See Dimethylglyoxime                                                                                                       |

**TABLE 11.20** Elements Precipitated by General Analytical Reagents (*Continued*)

| Reagent                                                                                                                    | Conditions                                                                                                                | Substances precipitated                                                                                                                                                                                              |
|----------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Diammonium hydrogen phosphate, $(\text{NH}_4)_2\text{HPO}_4$ (aqueous)                                                     | (a) Acid medium.<br>(b) Ammoniacal medium containing citrate or tartrate.                                                 | (a) <i>Bi, Co, Hf, In, Ti, Zn, Zr</i><br>(b) <i>Au, Ba, Be, Ca, Hg, In, La, Mg, Mn, Pb, rare earths, Sr, Th, U, Zr</i>                                                                                               |
| Dimethylglyoxime, $[\text{CH}_3\text{C}(\text{NOH})_2]$ (alcohol)                                                          | (a) Dilute $\text{HCl}$ or $\text{H}_2\text{SO}_4$ medium.<br>(b) Ammoniacal tartrate medium about pH 8. Weighed as such. | (a) <i>Au, Pd, Se</i><br>(b) <i>Ni</i> (and <i>Co, Fe</i> if present in large amounts)                                                                                                                               |
| Hydrazine, $\text{N}_2\text{H}_4$ (aqueous)                                                                                |                                                                                                                           | <i>Ag, Au, Cu, Hg, Ir, Os, Pd, Pt, Rh, Ru, Se, Te</i>                                                                                                                                                                |
| Hydrogen sulfide, $\text{H}_2\text{S}$                                                                                     | (a) $0.2\text{--}0.5M \text{H}^+$ .<br><br>(b) Ammoniacal solution after removal of acid sulfide group.                   | (a) <i>Ag, As, Au, Bi, Cd, Cu, Ge, Hg, In, Ir, Mo, Os, Pb, Pd, Pt, Re, Rh, Ru, Sb, Se, Sn, Te, Tl, V, W, Zn</i><br>(b) <i>Co, Fe, Ga, In, Mn, Ni, Tl, U, V, Zn</i>                                                   |
| 4-Hydroxyphenylarsonic acid, $\text{C}_6\text{H}_4(\text{OH})\text{AsO}(\text{OH})_2$ (aqueous)                            | Dilute acid solution.                                                                                                     | <i>Ce, Fe, Sn, Th, Ti, Zr</i>                                                                                                                                                                                        |
| 8-Hydroxyquinoline (oxine), $\text{C}_9\text{H}_6\text{NOH}$ , (alcohol)                                                   | (a) $\text{HOAc}\text{--}\text{OAc}^-$ buffer.<br><br>(b) Ammoniacal solution.                                            | (a) <i>Ag, Al, Bi, Cd, Co, Cr, Cu, Fe, Ga, Hg, In, La, Mn, Mo, Nb, Ni, Pb, Pd, rare earths, Sb, Ta, Th, Ti, V, W, Zn, Zr</i><br>(b) Same as in (a) except for <i>Ag</i> ; in addition, <i>Ba, Be, Ca, Mg, Sn, Sr</i> |
| 2-Mercaptobenzothiazole, $\text{C}_6\text{H}_4(\text{SCN})\text{SH}$ (acetic acid solution)                                | Ammoniacal solution, except for <i>Cu</i> , when a dilute acid solution is used.                                          | <i>Ag, Au, Bi, Cd, Cu, Hg, Ir, Pb, Pt, Rh, Tl</i>                                                                                                                                                                    |
| Nitron (diphenylenedianilohydrotriazole), $\text{C}_{20}\text{H}_{16}\text{N}_4$ , (5% acetic acid)                        | Dilute $\text{H}_2\text{SO}_4$ medium.                                                                                    | <i>B, ClO_3^-, ClO_4^-, NO_3^-, ReO_4^-, W</i>                                                                                                                                                                       |
| 1-Nitroso-2-naphthol, $\text{C}_{10}\text{H}_6(\text{NO})\text{OH}$ (very dilute alkali)                                   | Selective for <i>Co</i> ; acid solution. Precipitate ignited to $\text{Co}_3\text{O}_4$ .                                 | <i>Ag, Au, B, Co, Cr, Cu, Fe, Mo, Pd, Ti, V, W, Zr</i>                                                                                                                                                               |
| Oxalic acid, $\text{H}_2\text{C}_2\text{O}_4$ , (aqueous)                                                                  | Dilute acid solution.                                                                                                     | <i>Ag, Au, Cu, Hg, La, Ni, Pb, rare earths, Sc, Th, U(IV), W, Zr</i>                                                                                                                                                 |
| Phenylarsonic acid, $\text{C}_6\text{H}_5\text{AsO}(\text{OH})_2$ , (aqueous)                                              | Selective precipitants for quadrivalent metals in acid solution. Metals weighed as dioxides.                              | <i>Bi, Ce(IV), Fe, Hf, Mg, Sn, Ta, Th, Ti, U(IV), W, Zr</i>                                                                                                                                                          |
| Phenylthiohydantoic acid, $\text{C}_6\text{H}_5\text{N}=\text{C}(\text{NH}_2)\text{SCH}_2\text{COOH}$ (aqueous or alcohol) |                                                                                                                           | <i>Bi, Cd, Co, Cu, Fe, Hg, Ni, Pb, Sb</i>                                                                                                                                                                            |
| Picrolonic acid, $\text{C}_{10}\text{H}_7\text{O}_5\text{N}_4\text{H}$ (aqueous)                                           | Neutral solution.                                                                                                         | <i>Ca, Mg, Pb, Th</i>                                                                                                                                                                                                |
| Propylarsonic acid, $\text{C}_3\text{H}_9\text{AsO}(\text{OH})_2$ (aqueous)                                                | Preferred for <i>W</i> ; see Phenylarsonic acid.                                                                          |                                                                                                                                                                                                                      |
| Pyridine plus thiocyanate                                                                                                  | Dilute acid solution.                                                                                                     | <i>Ag, Cd, Cu, Mn, Ni</i>                                                                                                                                                                                            |
| Quinaldic acid, $\text{C}_9\text{H}_6\text{NCOOH}$ (aqueous)                                                               | Dilute acid solution.                                                                                                     | <i>Ag, Cd, Co, Cu, Fe, Hg, Mo, Ni, Pb, Pd, Pt(II), U, W, Zn</i>                                                                                                                                                      |
| Salicylaldoxime, $\text{C}_7\text{H}_5(\text{OH})\text{NOH}$ (alcohol)                                                     | Dilute acid solution.                                                                                                     | <i>Ag, Bi, Cd, Co, Cu, Fe, Hg, Mg, Mn, Ni, Pb, Pd, V, Zn</i>                                                                                                                                                         |
| Silver nitrate, $\text{AgNO}_3$ (aqueous)                                                                                  | (a) Dilute $\text{HNO}_3$ solution.<br>(b) Acetate buffer, pH 5–7.                                                        | (a) $\text{Br}^-, \text{Cl}^-, \text{I}^-, \text{SCN}^-$<br>(b) $\text{As(V)}, \text{CN}^-, \text{OCN}^-, \text{IO}_3^-, \text{Mo(VI)}, \text{N}_3^-, \text{S}^{2-}, \text{V(V)}$                                    |

**TABLE 11.20** Elements Precipitated by General Analytical Reagents (*Continued*)

| Reagent                                                                                                             | Conditions                                                                                                                                                                                | Substances precipitated                                                                                                                                         |
|---------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Sodium tetraphenylborate,<br>$\text{NaB}(\text{C}_6\text{H}_5)_4$ (aqueous)                                         | Specific for K group of alkali metals from dilute $\text{HNO}_3$ or $\text{HOAc}$ solution (pH 2), or pH 6.5 in presence of EDTA.                                                         | <i>Cs, K, <math>\text{NH}_4^+</math>, Rb</i>                                                                                                                    |
| Tannic acid (tannin), $\text{C}_{14}\text{H}_{10}\text{O}_9$ (aqueous)                                              | Acts as negative colloid that is a flocculent for positively charged hydrous oxide sols. Noteworthy for W in acid solution, and for Ta (from Nb in acidic oxalate medium).                | <i>Al, Be, Cr, Ga, Ge, Nb, Sb, Sn, Ta, Th, Ti, U, V, W, Zr</i>                                                                                                  |
| Tartaric acid,<br>$\text{HOOC}(\text{CHOH})_2\text{COOH}$ (aqueous)                                                 |                                                                                                                                                                                           | <i>Ca, K, Mg, Sc, Sr, Ta</i>                                                                                                                                    |
| Tetraphenylarsonium chloride,<br>$(\text{C}_6\text{H}_5)_4\text{AsCl}$ (aqueous)                                    | $(\text{C}_6\text{H}_5)_4\text{AsTiCl}_4$ and $(\text{C}_6\text{H}_5)_4\text{AsReO}_4$ weighed as such.                                                                                   | <i>Re, Tl</i>                                                                                                                                                   |
| Thioglycolic- $\beta$ -aminonaphthalide, thionalide,<br>$\text{C}_{10}\text{H}_7\text{NHCOCH}_2\text{SH}$ (alcohol) | (a) Acid solution.<br>(b) Carbonate medium containing tartrate.<br>(c) Carbonate medium containing tartrate and cyanide.<br>(d) Strongly alkaline medium containing tartrate and cyanide. | (a) <i>Ag, As, Au, Bi, Cu, Hg, Os, Pb, Pd, Rh, Ru, Sb, Sn, Tl</i><br>(b) <i>Au, Cd, Cu, Hg(II), Tl(I)</i><br>(c) <i>Au, Bi, Pb, Sb, Sn, Tl</i><br>(d) <i>Tl</i> |

**Source:** J. A. Dean, ed., *Analytical Chemistry Handbook*, McGraw-Hill, New York, 1995.

**TABLE 11.21** Cleaning Solutions for Fritted Glassware

| Material                         | Cleaning solution                                                                                                                                                                                           |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Fatty materials                  | Carbon tetrachloride.                                                                                                                                                                                       |
| Organic matter                   | Hot concentrated sulfuric acid plus a few drops of sodium or potassium nitrate solution.                                                                                                                    |
| Albumen                          | Hot aqueous ammonia or hot hydrochloric acid.                                                                                                                                                               |
| Glucose                          | Hot mixed acid (sulfuric plus nitric acids).                                                                                                                                                                |
| Copper or iron oxides            | Hot hydrochloric acid plus potassium chlorate.                                                                                                                                                              |
| Mercury residue                  | Not nitric acid.                                                                                                                                                                                            |
| Silver chloride                  | Aqueous ammonia or sodium thiosulfate.                                                                                                                                                                      |
| Aluminous and siliceous residues | A 2% hydrofluoric acid solution followed by concentrated sulfuric acid; rinse immediately with distilled water followed by a few milliliters of acetone. Repeat rinsing until all trace of acid is removed. |



TABLE 11.22 Common Fluxes

| Flux                                                                                                                                     | Melting point, °C | Types of crucible used for fusion                          | Type of substances decomposed                                                                               |
|------------------------------------------------------------------------------------------------------------------------------------------|-------------------|------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|
| Na <sub>2</sub> CO <sub>3</sub>                                                                                                          | 851               | Pt                                                         | For silicates, and silica-containing samples; alumina-containing samples; insoluble phosphates and sulfates |
| Na <sub>2</sub> CO <sub>3</sub> plus an oxidizing agent such as KNO <sub>3</sub> , KClO <sub>3</sub> , or Na <sub>2</sub> O <sub>2</sub> |                   | Pt (do not use with Na <sub>2</sub> O <sub>2</sub> ) or Ni | For samples needing an oxidizing agent                                                                      |
| NaOH or KOH                                                                                                                              | 320–380           | Au, Ag, Ni                                                 | For silicates, silicon carbide, certain minerals                                                            |
| Na <sub>2</sub> O <sub>2</sub>                                                                                                           | Decomposes        | Fe, Ni                                                     | For sulfides, acid-insoluble alloys of Fe, Ni, Cr, Mo, W, and Li; Pt alloys; Cr, Sn, Zn minerals            |
| K <sub>2</sub> S <sub>2</sub> O <sub>7</sub>                                                                                             | 300               | Pt or porcelain                                            | Acid flux for insoluble oxides and oxide-containing samples                                                 |
| B <sub>2</sub> O <sub>3</sub>                                                                                                            | 577               | Pt                                                         | For silicates and oxides when alkalis are to be determined                                                  |
| CaCO <sub>3</sub> plus NH <sub>4</sub> Cl                                                                                                |                   | Ni                                                         | For decomposing silicates in the determination of alkali element                                            |

TABLE 11.23 Membrane Filters

| Filter pore size, μm | Maximum rigid particle to penetrate, μm | Filter pore size, μm | Maximum rigid particle to penetrate, μm |
|----------------------|-----------------------------------------|----------------------|-----------------------------------------|
| 14                   | 17                                      | 0.65                 | 0.68                                    |
| 10                   | 12                                      | 0.60                 | 0.65                                    |
| 8                    | 9.4                                     | 0.45                 | 0.47                                    |
| 7                    | 9.0                                     | 0.30                 | 0.32                                    |
| 5                    | 6.2                                     | 0.22                 | 0.24                                    |
| 3                    | 3.9                                     | 0.20                 | 0.25                                    |
| 2                    | 2.5                                     | 0.10                 | 0.108                                   |
| 1.2                  | 1.5                                     | 0.05                 | 0.053                                   |
| 1.0                  | 1.1                                     | 0.025                | 0.028                                   |
| 0.8                  | 0.95                                    |                      |                                         |

**TABLE 11.24** Porosities of Fritted Glassware

| Porosity     | Nominal maximum pore size, $\mu\text{m}$ | Principal uses                                                                                                             |
|--------------|------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| Extra coarse | 170–220                                  | Filtration of very coarse materials. Gas dispersion, gas washing, and extractor beds. Support of other filter materials.   |
| Coarse       | 40–60                                    | Filtration of coarse materials. Gas dispersion, gas washing, gas absorption. Mercury filtration. For extraction apparatus. |
| Medium       | 10–15                                    | Filtration of crystalline precipitates. Removal of “floaters” from distilled water.                                        |
| Fine         | 4–5.5                                    | Filtration of fine precipitates. As a mercury valve. In extraction apparatus.                                              |
| Very fine    | 2–2.5                                    | General bacteria filtrations.                                                                                              |
| Ultra fine   | 0.9–1.4                                  | General bacteria filtrations.                                                                                              |

**TABLE 11.25** Tolerances for Analytical Weights

By Alan D. Westland with Fred E. Beamish.

This table gives the individual and group tolerances established by the National Bureau of Standards (Washington, D.C.) for classes M, S, S-1, and P weights. Individual tolerances are “acceptance tolerances” for new weights. Group tolerances are defined by the National Bureau of Standards as follows: “The corrections of individual weights shall be such that no combination of weights that is intended to be used in a weighing shall differ from the sum of the nominal values by more than the amount listed under the group tolerances.”

For class S-1 weights, two-thirds of the weights in a set must be within one-half of the individual tolerances given below. No group tolerances have been specified for class P weights. See *Natl. Bur. Standards Circ.* 547, sec. 1 (1954).

| Denomination | Class M                  |                     | Class S                  |                     | Class S-1, individual tolerance, mg | Class P, individual tolerance, mg |
|--------------|--------------------------|---------------------|--------------------------|---------------------|-------------------------------------|-----------------------------------|
|              | Individual tolerance, mg | Group tolerance, mg | Individual tolerance, mg | Group tolerance, mg |                                     |                                   |
| 100 g        | 0.50                     | None specified      | 0.25                     | None specified      | 1.0                                 | 2.0                               |
| 50 g         | 0.25                     |                     | 0.12                     |                     | 0.60                                | 1.2                               |
| 30 g         | 0.15                     |                     | 0.074                    |                     | 0.45                                | 0.90                              |
| 20 g         | 0.10                     |                     | 0.074                    |                     | 0.35                                | 0.70                              |
| 10 g         | 0.050                    |                     | 0.074                    |                     | 0.25                                | 0.50                              |
| 5 g          | 0.034                    | 0.065               | 0.054                    | 0.105               | 0.18                                | 0.36                              |
| 3 g          | 0.034                    |                     | 0.054                    |                     | 0.15                                | 0.14                              |
| 2 g          | 0.034                    |                     | 0.054                    |                     | 0.13                                | 0.26                              |
| 1 g          | 0.034                    |                     | 0.054                    |                     | 0.10                                | 0.20                              |
| 500 mg       | 0.0054                   | 0.0105              | 0.025                    | 0.055               | 0.080                               | 0.16                              |
| 300 mg       | 0.0054                   |                     | 0.025                    |                     | 0.070                               | 0.14                              |
| 200 mg       | 0.0054                   |                     | 0.025                    |                     | 0.060                               | 0.12                              |
| 100 mg       | 0.0054                   |                     | 0.025                    |                     | 0.050                               | 0.10                              |
| 50 mg        | 0.0054                   | 0.0105              | 0.014                    | 0.034               | 0.042                               | 0.085                             |
| 30 mg        | 0.0054                   |                     | 0.014                    |                     | 0.038                               | 0.076                             |
| 20 mg        | 0.0054                   |                     | 0.014                    |                     | 0.035                               | 0.070                             |

TABLE 11.25 Tolerances for Analytical Weights (Continued)

| Denomination | Class M                        |                           | Class S                        |                           | Class S-1,<br>individual<br>tolerance,<br>mg | Class P,<br>individual<br>tolerance,<br>mg |
|--------------|--------------------------------|---------------------------|--------------------------------|---------------------------|----------------------------------------------|--------------------------------------------|
|              | Individual<br>tolerance,<br>mg | Group<br>tolerance,<br>mg | Individual<br>tolerance,<br>mg | Group<br>tolerance,<br>mg |                                              |                                            |
| 10 mg        | 0.0054                         | 0.0105                    | 0.014                          | 0.034                     | 0.030                                        | 0.060                                      |
| 5 mg         | 0.0054                         |                           | 0.014                          |                           | 0.028                                        | 0.055                                      |
| 3 mg         | 0.0054                         |                           | 0.014                          |                           | 0.026                                        | 0.052                                      |
| 2 mg         | 0.0054                         |                           | 0.014                          |                           | 0.025                                        | 0.050                                      |
| 1 mg         | 0.0054                         |                           | 0.014                          |                           | 0.025                                        | 0.050                                      |
| ½ mg         | 0.0054                         |                           | 0.014                          |                           | 0.025                                        | .....                                      |

TABLE 11.26 Heating Temperatures, Composition of Weighing Forms, and Gravimetric Factors

The minimum temperature required for heating a pure precipitate to constant weight is frequently lower than that commonly recommended in gravimetric procedures. However, the higher temperature is very often still to be preferred in order to ensure that contaminating substances are expelled. The thermal stability ranges of various precipitates as deduced from thermograms are also tabulated. Where a stronger ignition is advisable, the safe upper limit can be ascertained.

Gravimetric factors are based on the 1993 International Atomic Weights. The factor Ag: 0.7526 given in the first line of the table indicates that the weight of precipitate obtained (AgCl) is to be multiplied by 0.7526 to calculate the corresponding weight of silver.

| Element | Thermal stability<br>range, °C | Final heating<br>temperature, °C | Composition of<br>weighing form                                  | Gravimetric factors                                 |
|---------|--------------------------------|----------------------------------|------------------------------------------------------------------|-----------------------------------------------------|
| Ag      | 70–600                         | 130–150                          | AgCl                                                             | Ag: 0.7526                                          |
| Al      | > 475                          | 1200                             | Al <sub>2</sub> O <sub>3</sub>                                   | Al: 0.5293                                          |
|         | > 743                          | > 743                            | AlPO <sub>4</sub>                                                | Al: 0.2212; Al <sub>2</sub> O <sub>3</sub> : 0.4180 |
| As      | 102–220                        | 110                              | Al(C <sub>9</sub> H <sub>6</sub> NO) <sub>3</sub>                | Al: 0.0587; Al <sub>2</sub> O <sub>3</sub> : 0.1110 |
|         | 200–275                        | 105–110                          | Al <sub>2</sub> S <sub>3</sub>                                   | As: 0.6090; As <sub>2</sub> O <sub>3</sub> : 0.8041 |
|         |                                | 850                              | Mg <sub>2</sub> As <sub>2</sub> O <sub>7</sub>                   | As: 0.4827; As <sub>2</sub> O <sub>3</sub> : 0.6373 |
|         |                                | vacuum at 25                     | MgNH <sub>4</sub> AsO <sub>4</sub> · 6H <sub>2</sub> O           | As: 0.2589                                          |
| Au      | 20–957                         | 1060                             | Au                                                               |                                                     |
| Ba      | 780–1100                       | 780                              | BaSO <sub>4</sub>                                                | Ba: 0.5884; BaO: 0.6570                             |
|         | < 60                           | < 60                             | BaCrO <sub>4</sub>                                               | Ba: 0.5421; BaO: 0.6053                             |
| Be      | > 900                          | 1000                             | BeO                                                              | Be: 0.3603                                          |
| Bi      |                                | 100                              | BiOCl                                                            | Bi: 0.8024; Bi <sub>2</sub> O <sub>3</sub> : 0.8946 |
|         |                                | 100                              | Bi(C <sub>12</sub> H <sub>10</sub> NOS) <sub>3</sub>             | Bi: 0.2387                                          |
|         |                                | 800                              | BiPO <sub>4</sub>                                                | Bi: 0.6875; Bi <sub>2</sub> O <sub>3</sub> : 0.7665 |
| Br      | 70–946                         | 130–150                          | AgBr                                                             | Br: 0.4256                                          |
| Ca      | 478–635                        | 475–525                          | CaCO <sub>3</sub>                                                | Ca: 0.4004; CaO: 0.5601                             |
|         | 838–1025                       | 950–1000                         | CaO                                                              | Ca: 0.7147                                          |
| Cd      |                                | air-dried                        | Ca(picrolonate) <sub>2</sub> · 8H <sub>2</sub> O                 | Ca: 0.05642                                         |
|         |                                | > 320                            | CdSO <sub>4</sub>                                                | Cd: 0.5392; CdO: 0.6159                             |
|         |                                | 125                              | Cd(C <sub>10</sub> H <sub>6</sub> NO <sub>2</sub> ) <sub>2</sub> | Cd: 0.2462                                          |
| Ce      | 218–420                        |                                  | CdS                                                              | Cd: 0.7781; CdO: 0.8888                             |
|         | > 360                          | 500–600                          | CeO <sub>2</sub>                                                 | Ce: 0.8141                                          |
| Cl      | 70–600                         | 130–150                          | AgCl                                                             | Cl: 0.2474                                          |

**TABLE 11.26** Heating Temperatures, Composition of Weighing Forms, and Gravimetric Factors (*Continued*)

| Element                              | Thermal stability range, °C | Final heating temperature, °C | Composition of weighing form                                                                                            | Gravimetric factors                                           |
|--------------------------------------|-----------------------------|-------------------------------|-------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------|
| Co                                   | 285–946                     | 750–850                       | Co <sub>3</sub> O <sub>4</sub>                                                                                          | Co: 0.7342                                                    |
|                                      |                             | 130                           | Co(C <sub>10</sub> H <sub>6</sub> NO <sub>2</sub> ) <sub>3</sub> · 2H <sub>2</sub> O                                    | Co: 0.09639; CoO: 0.1226                                      |
|                                      |                             | 450–500                       | CoSO <sub>4</sub>                                                                                                       | Co: 0.3802                                                    |
| Cr                                   |                             | 120                           | PbCrO <sub>4</sub>                                                                                                      | Cr: 0.1609                                                    |
| Cu                                   |                             | 105–120                       | CuSCN                                                                                                                   | Cu: 0.5225; CuO: 0.6540                                       |
|                                      | < 115                       | 100–105                       | Cu(C <sub>7</sub> H <sub>5</sub> NO <sub>2</sub> ) <sub>2</sub>                                                         | Cu: 0.1891                                                    |
|                                      |                             | 105–115                       | Cu(C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub> )                                                                    | Cu: 0.2201                                                    |
|                                      |                             | 110–115                       | Cu(C <sub>10</sub> H <sub>6</sub> NO <sub>2</sub> ) · H <sub>2</sub> O                                                  | Cu: 0.1494                                                    |
|                                      |                             | 105                           | Cu(C <sub>12</sub> H <sub>10</sub> NOS) <sub>2</sub> · H <sub>2</sub> O                                                 | Cu: 0.1237                                                    |
| F                                    | 66–538                      | 130–140                       | PbClF                                                                                                                   | F: 0.07261                                                    |
| Fe                                   | 470–946                     | 900                           | Fe <sub>2</sub> O <sub>3</sub>                                                                                          | Fe: 0.6994                                                    |
| Ga                                   | 408–946                     | 900                           | Ga <sub>2</sub> O <sub>3</sub>                                                                                          | Ga: 0.7439                                                    |
| Hg                                   |                             | 105                           | Hg(C <sub>12</sub> H <sub>10</sub> NOS) <sub>2</sub>                                                                    | Hg: 0.3169                                                    |
| I                                    | 60–900                      | 130–150                       | AgI                                                                                                                     | I: 0.5405                                                     |
| In                                   | 345–1200                    | 1200                          | In <sub>2</sub> O <sub>3</sub>                                                                                          | In: 0.8271                                                    |
| Ir                                   |                             |                               | IrO <sub>2</sub>                                                                                                        | Ir: 0.8573                                                    |
| K                                    | 73–653                      | < 653                         | KClO <sub>4</sub>                                                                                                       | K: 0.2822; K <sub>2</sub> O: 0.3399                           |
|                                      |                             | < 270                         | K <sub>2</sub> PtCl <sub>6</sub>                                                                                        | K: 0.1609; K <sub>2</sub> O: 0.1938                           |
|                                      |                             |                               | KIO <sub>4</sub>                                                                                                        | K: 0.1700                                                     |
|                                      |                             | 120                           | KB(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>                                                                         | K: 0.1091                                                     |
| Li                                   |                             | 200                           | Li <sub>2</sub> SO <sub>4</sub>                                                                                         | Li: 0.1263; Li <sub>2</sub> O: 0.2718                         |
| Mg                                   |                             | 1050–1100                     | Mg <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                                                                           | Mg: 0.2184; MgO: 0.3622                                       |
|                                      | 88–300                      | 155–160                       | Mg(C <sub>9</sub> H <sub>6</sub> NO) <sub>2</sub>                                                                       | Mg: 0.07775; MgO: 0.1289                                      |
| Mn                                   | > 946                       | 1000                          | Mn <sub>3</sub> O <sub>4</sub>                                                                                          | Mn: 0.7203                                                    |
|                                      |                             | 1000                          | Mn <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                                                                           | Mn: 0.3871; MnO: 0.4998                                       |
| Mo                                   |                             | > 505                         | PbMoO <sub>4</sub>                                                                                                      | Mo: 0.2613; MoO <sub>3</sub> : 0.3291                         |
|                                      |                             | 500–525                       | MoO <sub>3</sub>                                                                                                        | Mo: 0.6666                                                    |
| N (as NO <sub>3</sub> <sup>-</sup> ) | 20–242                      | 105                           | Nitron nitrate                                                                                                          | N: 0.3732; NO <sub>3</sub> : 0.1652                           |
| Na                                   | 360–674                     | 125                           | NaMg(UO <sub>2</sub> ) <sub>3</sub> (C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ) <sub>9</sub> · 6.5 H <sub>2</sub> O | Na: 0.01527; Na <sub>2</sub> O: 0.02058                       |
| Nb                                   | 650–950                     | 900                           | Nb <sub>2</sub> O <sub>3</sub>                                                                                          | Nb: 0.6990                                                    |
| Ni                                   | 79–172                      | 110–120                       | Ni(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub>                                           | Ni: 0.2032; NiO: 0.2586                                       |
| Os                                   |                             | 800 (in H <sub>2</sub> )      | Os metal                                                                                                                |                                                               |
| P                                    |                             | > 477                         | Mg <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                                                                           | P: 0.2783; PO <sub>4</sub> : 0.8536                           |
|                                      | 160–415                     | 110                           | (NH <sub>4</sub> ) <sub>3</sub> [P(Mo <sub>3</sub> O <sub>10</sub> ) <sub>4</sub> ]                                     | P: 0.0165; P <sub>2</sub> O <sub>5</sub> : 0.0378             |
| Pb                                   | 271–959                     | 500–600                       | PbSO <sub>4</sub>                                                                                                       | Pb: 0.6832; PbO: 0.7359                                       |
|                                      |                             | 600                           | PbMoO <sub>4</sub>                                                                                                      | Pb: 0.5643; PbO: 0.6078                                       |
|                                      |                             | 120                           | PbCrO <sub>4</sub>                                                                                                      | Pb: 0.6411                                                    |
|                                      | 271–959                     | 600–800                       | PbSO <sub>4</sub>                                                                                                       | Pb: 0.6832; PbO: 0.7359                                       |
|                                      |                             | 105                           | Pb(C <sub>12</sub> H <sub>10</sub> NOS) <sub>2</sub>                                                                    | Pb: 0.3240                                                    |
| Pd                                   | 45–171                      | 110                           | Pd(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub>                                           | Pd: 0.3162                                                    |
| Rb                                   | 70–674                      | < 674                         | Rb <sub>2</sub> PtCl <sub>6</sub>                                                                                       | Rb: 0.2954; Rb <sub>2</sub> O: 0.3230                         |
| Re                                   |                             | 130                           | (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> AsReO <sub>4</sub>                                                        | Re: 0.2939                                                    |
|                                      |                             | 110                           | Nitron perhenate                                                                                                        | Re: 0.3306                                                    |
| S                                    |                             | > 780                         | BaSO <sub>4</sub>                                                                                                       | S: 0.1374; SO <sub>3</sub> : 0.3430; SO <sub>4</sub> : 0.4116 |
| Sb                                   |                             | 100                           | Sb(C <sub>12</sub> H <sub>10</sub> NOS) <sub>3</sub>                                                                    | Sb: 0.1581                                                    |
| SCN <sup>-</sup>                     |                             | 130                           | AgSCN                                                                                                                   | SCN: 0.3500                                                   |
|                                      |                             | 110–120                       | CuSCN                                                                                                                   | SCN: 0.4775                                                   |
| Se                                   |                             | 120–130                       | Se metal                                                                                                                | SeO <sub>2</sub> : 1.4052                                     |
| Si                                   | 358–946                     | > 358                         | SiO <sub>2</sub>                                                                                                        | Si: 0.4675                                                    |

**TABLE 11.26** Heating Temperatures, Composition of Weighing Forms, and Gravimetric Factors (*Continued*)

| Element | Thermal stability range, °C | Final heating temperature, °C | Composition of weighing form                                                        | Gravimetric factors                   |
|---------|-----------------------------|-------------------------------|-------------------------------------------------------------------------------------|---------------------------------------|
| Sn      | > 834                       | 900                           | SnO <sub>2</sub>                                                                    | Sn: 0.7877                            |
| Sr      |                             | 130–140                       | Sr(NO <sub>3</sub> ) <sub>2</sub>                                                   | Sr: 0.4140                            |
|         | 100–300                     | 100–300                       | SrSO <sub>4</sub>                                                                   | Sr: 0.4770; SrO: 0.5641               |
| Te      |                             | 105                           | Te metal                                                                            |                                       |
| Th      | 610–946                     | 700–800                       | ThO <sub>2</sub>                                                                    | Th: 0.8788                            |
|         |                             | 900                           | ThP <sub>2</sub> O <sub>7</sub>                                                     | Th: 0.5863                            |
| Ti      | 350–946                     | 900                           | TiO <sub>2</sub>                                                                    | Ti: 0.5992                            |
| Tl(III) |                             | 100                           | Tl(C <sub>12</sub> H <sub>10</sub> NOS)                                             | Tl: 0.4860                            |
| U       |                             | 1000                          | U <sub>3</sub> O <sub>8</sub>                                                       | U: 0.8480; UO <sub>2</sub> : 0.9620   |
| V       | 581–946                     | 700–800                       | V <sub>2</sub> O <sub>5</sub>                                                       | V: 0.5602                             |
| W       | > 674                       | 800–900                       | WO <sub>3</sub>                                                                     | W: 0.7930                             |
| Zn      | > 1000                      | 950–1000                      | ZnO                                                                                 | Zn: 0.8034                            |
|         |                             | 1000                          | Zn <sub>2</sub> P <sub>2</sub> O <sub>7</sub>                                       | Zn: 0.4292; ZnO: 0.5342               |
|         |                             | 125                           | Zn(C <sub>10</sub> H <sub>6</sub> NO <sub>2</sub> ) <sub>2</sub> · H <sub>2</sub> O | Zn: 0.1529                            |
| Zr      |                             | > 850                         | ZrP <sub>2</sub> O <sub>7</sub>                                                     | Zr: 0.3440; ZrO <sub>2</sub> : 0.4647 |
|         |                             | 1200                          | ZrO <sub>2</sub>                                                                    | Zr: 0.7403                            |

Source: J. A. Dean, ed., *Analytical Chemistry Handbook*, McGraw-Hill, New York, 1995.

11.6 VOLUMETRIC ANALYSIS

11.6.1 Acid-Base Titrations in Aqueous Media

**TABLE 11.27** Primary Standards for Aqueous Acid-Base Titrations

| Standard                                                           | Formula weight | Preparation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|--------------------------------------------------------------------|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Basic substances for standardizing acidic solutions                |                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| (HOCH <sub>2</sub> ) <sub>3</sub> CNHH <sub>2</sub>                | 121.137        | Tris(hydroxymethyl)aminomethane is available commercially as a primary standard. Dry at 100–103°C (<110°C). In titrations with a strong acid the equivalence point is at about pH 4.5–5. Equivalent weight is the formula weight. [J. H. Fossum, P. C. Markunas, and J. A. Riddick, <i>Anal. Chem.</i> , <b>23</b> :491 (1951).]                                                                                                                                                               |
| HgO                                                                | 216.59         | Dissolve 100 g pure HgCl <sub>2</sub> in 1 L H <sub>2</sub> O, and add with stirring to 650 mL 1.5 M NaOH. Filter and wash with H <sub>2</sub> O until washings are neutral to phenolphthalein. Dry to constant weight at or below 40°C, and store in a dark bottle. To 0.4 g HgO (≡ 40 mL 0.1N acid) add 10–15 g KBr plus 20–25 mL H <sub>2</sub> O. Stir, excluding CO <sub>2</sub> , until solution is complete. Titrate with acid to pH 5–8. Equivalent weight is one-half formula weight. |
| Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> · 10H <sub>2</sub> O | 381.372        | Recrystallize reagent-grade salt twice from water at temperatures below 55°C. Wash the crystals with H <sub>2</sub> O, twice with ethanol, and twice with diethyl ether. Let stand in a hygrostat oversaturated NaBr · 2H <sub>2</sub> O or saturated NaCl-sucrose solution. Use methyl red indicator. Equivalent weight is one-half the formula weight.                                                                                                                                       |

**TABLE 11.27** Primary Standards for Aqueous Acid-Base Titrations (*Continued*)

| Standard                                                                 | Formula weight | Preparation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|--------------------------------------------------------------------------|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Basic substances for standardizing acidic solutions ( <i>continued</i> ) |                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Na <sub>2</sub> CO <sub>3</sub>                                          | 105.989        | Heat reagent-grade material for 1 hr at 255–265°C. Cool in an efficient desiccator. Titrate sample with acid to pH 4–5 (first green tint of bromocresol green), boil the solution to eliminate the carbon dioxide, cool, and again titrate to pH 4–5. Equivalent weight is one-half the formula weight.                                                                                                                                                                                              |
| NaCl                                                                     | 58.45          | Accurately weigh about 6 g NaCl and dissolve in distilled water. Pass the solution through a well-rinsed cation exchange column (Dowex 50W) in the hydrogen form. The equivalent amount of HCl is washed from the column (in 10 column volumes) into a volumetric flask and made up to volume. Equivalent weight is the formula weight.                                                                                                                                                              |
| Acidic substances for standardizing basic solutions                      |                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| C <sub>6</sub> H <sub>5</sub> COOH                                       | 122.125        | Pure benzoic acid is available from NIST (National Institute for Science and Technology). Dissolve 0.5 g in 20 mL of neutral ethanol (run a blank), excluding CO <sub>2</sub> , add 20–50 mL, and titrate using phenolphthalein as indicator.                                                                                                                                                                                                                                                        |
| <i>o</i> -C <sub>6</sub> H <sub>4</sub> (COOK)(COOH)                     | 204.22         | Potassium hydrogen <i>o</i> -phthalate is available commercially as primary standard, also from NIST. Dry at <135°C. Dissolve in water, excluding CO <sub>2</sub> , and titrate with phenolphthalein as indicator. For Ba(OH) <sub>2</sub> solution, perform the titration at an elevated temperature to prevent precipitation of Ba phthalate.                                                                                                                                                      |
| KH(IO <sub>3</sub> ) <sub>2</sub>                                        | 389.915        | Potassium hydrogen bis(iodate) is available commercially in a primary standard grade. Dry at 110°C. Dissolve a weighed amount of the salt in water, excluding CO <sub>2</sub> , and titrate to pH 5–8. [I. M. Kolthoff and L. H. van Berk, <i>J. Am. Chem. Soc.</i> , <b>48</b> :2800 (1926)].                                                                                                                                                                                                       |
| NH <sub>2</sub> SO <sub>3</sub> H                                        | 97.09          | Hydrogen amidosulfate (sulfamic acid) acts as a strong acid. Primary standard grade is available commercially. Since it does undergo slow hydrolysis, an acid end point (pH 4 to 6.5) should be chosen unless fresh reagent is available, then the end point can be in the range pH 4 to 9. [W. F. Wagner, J. A. Wuellner, and C. E. Feiler, <i>Anal. Chem.</i> , <b>24</b> :1491 (1952). M. J. Butler, G. F. Smith, and L. F. Audrieth, <i>Ind. Eng. Chem., Anal. Ed.</i> , <b>10</b> :690 (1938)]. |

TABLE 11.28 Titrimetric (Volumetric) Factors

| Acids                                                                                                                                                                                                                                  |                                                                    |          |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------|----------|
| The following factors are the equivalent of 1 mL of <i>normal acid</i> . Where the normality of the solution being used is other than normal, multiply the factors given in the table below by the normality of the solution employed. |                                                                    |          |
| The equivalents of the esters are based on the results of saponification.                                                                                                                                                              |                                                                    |          |
| The indicators methyl orange and phenolphthalein are indicated by the abbreviations MO and pH, respectively.                                                                                                                           |                                                                    |          |
| Substance                                                                                                                                                                                                                              | Formula                                                            | Grams    |
| Ammonia                                                                                                                                                                                                                                | NH <sub>3</sub>                                                    | 0.017031 |
| Ammonium                                                                                                                                                                                                                               | NH <sub>4</sub>                                                    | 0.018039 |
| Ammonium chloride                                                                                                                                                                                                                      | NH <sub>4</sub> Cl                                                 | 0.053492 |
| Ammonium hydroxide                                                                                                                                                                                                                     | NH <sub>4</sub> OH                                                 | 0.035046 |
| Ammonium oleate                                                                                                                                                                                                                        | C <sub>17</sub> H <sub>33</sub> CO <sub>2</sub> NH <sub>4</sub>    | 0.29950  |
| Ammonium oxide                                                                                                                                                                                                                         | (NH <sub>4</sub> ) <sub>2</sub> O                                  | 0.026038 |
| Amyl acetate                                                                                                                                                                                                                           | CH <sub>3</sub> CO <sub>2</sub> C <sub>5</sub> H <sub>11</sub>     | 0.13019  |
| Barium carbonate (MO)                                                                                                                                                                                                                  | BaCO <sub>3</sub>                                                  | 0.09867  |
| Barium hydroxide                                                                                                                                                                                                                       | Ba(OH) <sub>2</sub>                                                | 0.085677 |
| Barium oxide                                                                                                                                                                                                                           | BaO                                                                | 0.07667  |
| Bornyl acetate                                                                                                                                                                                                                         | CH <sub>3</sub> CO <sub>2</sub> C <sub>10</sub> H <sub>17</sub>    | 0.19629  |
| Calcium carbonate (MO)                                                                                                                                                                                                                 | CaCO <sub>3</sub>                                                  | 0.05004  |
| Calcium hydroxide                                                                                                                                                                                                                      | Ca(OH) <sub>2</sub>                                                | 0.037047 |
| Calcium oleate                                                                                                                                                                                                                         | (C <sub>17</sub> H <sub>33</sub> CO <sub>2</sub> ) <sub>2</sub> Ca | 0.30150  |
| Calcium oxide                                                                                                                                                                                                                          | CaO                                                                | 0.02804  |
| Calcium stearate                                                                                                                                                                                                                       | (C <sub>17</sub> H <sub>35</sub> CO <sub>2</sub> ) <sub>2</sub> Ca | 0.30352  |
| Casein (N 6.38)                                                                                                                                                                                                                        | .....                                                              | 0.089371 |
| Ethyl acetate                                                                                                                                                                                                                          | CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>      | 0.088107 |
| Glue (N 5.60)                                                                                                                                                                                                                          | .....                                                              | 0.078445 |
| Hydrochloric acid                                                                                                                                                                                                                      | HCl                                                                | 0.036461 |
| Magnesium carbonate (MO)                                                                                                                                                                                                               | MgCO <sub>3</sub>                                                  | 0.04216  |
| Magnesium oxide                                                                                                                                                                                                                        | MgO                                                                | 0.02016  |
| Menthyl acetate                                                                                                                                                                                                                        | CH <sub>3</sub> CO <sub>2</sub> C <sub>10</sub> H <sub>19</sub>    | 0.19831  |
| Methyl acetate                                                                                                                                                                                                                         | CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>                    | 0.074080 |
| Nicotine                                                                                                                                                                                                                               | C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>                     | 0.16224  |
| Nitrogen                                                                                                                                                                                                                               | N                                                                  | 0.014007 |
| Potassium carbonate (MO)                                                                                                                                                                                                               | K <sub>2</sub> CO <sub>3</sub>                                     | 0.06911  |
| Potassium carbonate, acid (MO)                                                                                                                                                                                                         | KHCO <sub>3</sub>                                                  | 0.10012  |
| Potassium nitrate                                                                                                                                                                                                                      | KNO <sub>3</sub>                                                   | 0.10111  |
| Potassium oleate                                                                                                                                                                                                                       | C <sub>17</sub> H <sub>33</sub> CO <sub>2</sub> K                  | 0.32057  |
| Potassium oxide                                                                                                                                                                                                                        | K <sub>2</sub> O                                                   | 0.04710  |
| Potassium stearate                                                                                                                                                                                                                     | C <sub>17</sub> K <sub>35</sub> CO <sub>2</sub> K                  | 0.32258  |
| Protein (N 5.70)                                                                                                                                                                                                                       | .....                                                              | 0.079846 |
| Protein (N 6.25)                                                                                                                                                                                                                       | .....                                                              | 0.087550 |
| Sodium acetate                                                                                                                                                                                                                         | CH <sub>3</sub> CO <sub>2</sub> Na                                 | 0.082035 |
| Sodium acetate                                                                                                                                                                                                                         | CH <sub>3</sub> CO <sub>2</sub> Na·3H <sub>2</sub> O               | 0.13608  |
| Sodium borate, tetra- (MO)                                                                                                                                                                                                             | Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>                      | 0.10061  |
| Sodium borate, tetra- (MO)                                                                                                                                                                                                             | Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O  | 0.19069  |
| Sodium carbonate (MO)                                                                                                                                                                                                                  | Na <sub>2</sub> CO <sub>3</sub>                                    | 0.052994 |
| Sodium carbonate (MO)                                                                                                                                                                                                                  | Na <sub>2</sub> CO <sub>3</sub> ·H <sub>2</sub> O                  | 0.062002 |
| Sodium carbonate (MO)                                                                                                                                                                                                                  | Na <sub>2</sub> CO <sub>3</sub> ·10H <sub>2</sub> O                | 0.14307  |
| Sodium carbonate, acid (MO)                                                                                                                                                                                                            | NaHCO <sub>3</sub>                                                 | 0.084007 |
| Sodium hydroxide                                                                                                                                                                                                                       | NaOH                                                               | 0.39997  |
| Sodium oleate                                                                                                                                                                                                                          | C <sub>17</sub> H <sub>33</sub> CO <sub>2</sub> Na                 | 0.30445  |

**TABLE 11.28** Titrimetric (Volumetric) Factors (*Continued*)

| Acids ( <i>continued</i> ) |                                                              |          |
|----------------------------|--------------------------------------------------------------|----------|
| Substance                  | Formula                                                      | Grams    |
| Sodium oxalate             | $\text{Na}_2\text{C}_2\text{O}_4$                            | 0.067000 |
| Sodium oxide               | $\text{Na}_2\text{O}$                                        | 0.030990 |
| Sodium phosphate (MO)      | $\text{Na}_2\text{HPO}_4$                                    | 0.14196  |
| Sodium phosphate (MO)      | $\text{Na}_2\text{P}_2\text{O}_7 \cdot 12\text{H}_2\text{O}$ | 0.35814  |
| Sodium phosphate (MO)      | $\text{Na}_3\text{PO}_4$                                     | 0.081970 |
| Sodium phosphate (PH)      | $\text{Na}_3\text{PO}_4$                                     | 0.16394  |
| Sodium silicate            | $\text{Na}_2\text{Si}_4\text{O}_9$                           | 0.15111  |
| Sodium stearate            | $\text{C}_{17}\text{H}_{35}\text{CO}_2\text{Na}$             | 0.30647  |
| Sodium sulfide (MO)        | $\text{Na}_2\text{S}$                                        | 0.039022 |
| Alkali                     |                                                              |          |

The following factors are the equivalent of the milliliter of *normal alkali*. Where the normality of the solution being used is other than normal, multiply the factors given in the table below by the normality of the solution employed.

The equivalents of the esters are based on the results of saponification.

The indicators methyl orange and phenolphthalein are indicated by the abbreviations MO and PH, respectively.

| Substance                 | Formula                                                             | Grams    |
|---------------------------|---------------------------------------------------------------------|----------|
| Abietic acid (PH)         | $\text{HC}_{20}\text{H}_{29}\text{O}_2$                             | 0.30246  |
| Acetic acid (PH)          | $\text{CH}_3\text{CO}_2\text{H}$                                    | 0.06005  |
| Acetic anhydride (PH)     | $(\text{CH}_3\text{CO})_2\text{O}$                                  | 0.051045 |
| Aluminum sulfate          | $\text{Al}_2(\text{SO}_4)_3$                                        | 0.05702  |
| Amyl acetate              | $\text{CH}_3\text{CO}_2\text{C}_5\text{H}_{11}$                     | 0.13019  |
| Benzoic acid (PH)         | $\text{C}_6\text{H}_5\text{CO}_2\text{H}$                           | 0.12212  |
| Borate tetra- (PH)        | $\text{B}_4\text{O}_7$                                              | 0.03881  |
| Boric acid (PH)           | $\text{H}_3\text{BO}_3$                                             | 0.061833 |
| Boric anhydride (PH)      | $\text{B}_2\text{O}_3$                                              | 0.03486  |
| Bornyl acetate            | $\text{CH}_3\text{CO}_2\text{C}_{10}\text{H}_{17}$                  | 0.19629  |
| Butyric acid (PH)         | $\text{C}_3\text{H}_7\text{CO}_2\text{H}$                           | 0.088107 |
| Calcium acetate           | $(\text{CH}_3\text{CO}_2)_2\text{Ca}$                               | 0.079085 |
| Calcium oleate            | $(\text{C}_{17}\text{H}_{33}\text{CO}_2)_2\text{Ca}$                | 0.30150  |
| Calcium stearate          | $(\text{C}_{17}\text{H}_{35}\text{CO}_2)_2\text{Ca}$                | 0.30352  |
| Carbon dioxide (PH)       | $\text{CO}_2$                                                       | 0.022005 |
| Chlorine                  | $\text{Cl}$                                                         | 0.035453 |
| Citric acid (PH)          | $\text{H}_3\text{C}_6\text{H}_5\text{O}_7 \cdot \text{H}_2\text{O}$ | 0.070047 |
| Ethyl acetate             | $\text{CH}_3\text{CO}_2\text{C}_2\text{H}_5$                        | 0.088107 |
| Formaldehyde              | $\text{HCHO}$                                                       | 0.030026 |
| Formic acid (PH)          | $\text{HCO}_2\text{H}$                                              | 0.046026 |
| Glycerol (sap. of acetyl) | $\text{C}_3\text{H}_5(\text{OH})_3$                                 | 0.030698 |
| Hydriodic acid            | $\text{HI}$                                                         | 0.12791  |
| Hydrobromic acid          | $\text{HBr}$                                                        | 0.080917 |
| Hydrochloric acid         | $\text{HCl}$                                                        | 0.036461 |
| Lactic acid (PH)          | $\text{HC}_3\text{H}_5\text{O}_3$                                   | 0.090079 |
| Lead acetate              | $(\text{CH}_3\text{CO}_2)_2\text{Pb} \cdot 3\text{H}_2\text{O}$     | 0.18966  |
| Maleic acid (PH)          | $(\text{CHCO}_2\text{H})_2$                                         | 0.058037 |
| Malic acid (PH)           | $\text{H}_2\text{C}_4\text{H}_4\text{O}_5$                          | 0.067045 |
| Menthol (sap. of acetyl)  | $\text{C}_{10}\text{H}_{19}\text{OH}$                               | 0.15627  |



TABLE 11.28 Titrimetric (Volumetric) Factors (Continued)

| Alkali (continued)             |                                                                     |          |
|--------------------------------|---------------------------------------------------------------------|----------|
| Substance                      | Formula                                                             | Grams    |
| Menthyl acetate                | $\text{CH}_3\text{CO}_2\text{C}_{10}\text{H}_{19}$                  | 0.19831  |
| Methyl acetate                 | $\text{CH}_3\text{CO}_2\text{CH}_3$                                 | 0.074080 |
| Nitrate                        | $\text{NO}_3$                                                       | 0.062005 |
| Nitric acid                    | $\text{HNO}_3$                                                      | 0.063013 |
| Nitrogen                       | $\text{N}$                                                          | 0.014007 |
| Nitrogen pentoxide             | $\text{N}_2\text{O}_5$                                              | 0.054005 |
| Oleic acid (PH)                | $\text{C}_{17}\text{H}_{33}\text{CO}_2\text{H}$                     | 0.28247  |
| Oxalic acid (PH)               | $(\text{CO}_2\text{H})_2$                                           | 0.045018 |
| Oxalic acid (PH)               | $(\text{CO}_2\text{H})_2 \cdot 2\text{H}_2\text{O}$                 | 0.063033 |
| Phosphoric acid (MO)           | $\text{H}_3\text{PO}_4$                                             | 0.097995 |
| Phosphoric acid (PH)           | $\text{H}_3\text{PO}_4$                                             | 0.048998 |
| Potassium carbonate, acid (MO) | $\text{KHCO}_3$                                                     | 0.10012  |
| Potassium oleate               | $\text{C}_{17}\text{K}_{33}\text{CO}_2\text{K}$                     | 0.32056  |
| Potassium oxalate, acid (PH)   | $\text{KHC}_2\text{O}_4$                                            | 0.12813  |
| Potassium phthalate, acid (PH) | $\text{HC}_8\text{H}_4\text{O}_4\text{K}$                           | 0.20423  |
| Potassium stearate             | $\text{C}_{17}\text{H}_{35}\text{CO}_2\text{K}$                     | 0.32258  |
| Sodium benzoate                | $\text{C}_6\text{H}_5\text{CO}_2\text{Na}$                          | 0.14411  |
| Sodium borate, tetra- (PH)     | $\text{Na}_2\text{B}_4\text{O}_7$                                   | 0.050305 |
| Sodium borate, tetra- (PH)     | $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$        | 0.095343 |
| Sodium carbonate, acid (MO)    | $\text{NaHCO}_3$                                                    | 0.084007 |
| Sodium oleate                  | $\text{C}_{17}\text{H}_{33}\text{CO}_2\text{Na}$                    | 0.30445  |
| Sodium salicylate              | $\text{C}_6\text{H}_5\text{OCO}_2\text{Na}$                         | 0.16011  |
| Stearic acid (PH)              | $\text{C}_{17}\text{H}_{35}\text{CO}_2\text{H}$                     | 0.28449  |
| Succinic acid (PH)             | $(\text{CH}_2\text{CO}_2\text{H})_2$                                | 0.059045 |
| Sulfate                        | $\text{SO}_4$                                                       | 0.048031 |
| Sulfur dioxide (PH)            | $\text{SO}_2$                                                       | 0.032031 |
| Sulfur trioxide                | $\text{SO}_3$                                                       | 0.040031 |
| Sulfuric acid                  | $\text{H}_2\text{SO}_4$                                             | 0.049039 |
| Sulfurous acid (PH)            | $\text{H}_2\text{SO}_3$                                             | 0.041039 |
| Tartaric acid (PH)             | $\text{H}_2\text{C}_4\text{H}_4\text{O}_6$                          | 0.075044 |
| Tartaric acid (PH)             | $\text{H}_2\text{C}_4\text{H}_4\text{O}_6 \cdot \text{H}_2\text{O}$ | 0.084052 |

Iodine

The following factors are the equivalent of 1 mL of *normal iodine*. Where the normality of the solution being used is other than normal, multiply the factors given in the table below by the normality of the solution employed.

| Substance         | Formula                       | Grams     |
|-------------------|-------------------------------|-----------|
| Acetone           | $(\text{CH}_3)_2\text{CO}$    | 0.0096801 |
| Ammonium chromate | $(\text{NH}_4)_2\text{CrO}_4$ | 0.050690  |
| Antimony          | $\text{Sb}$                   | 0.06088   |
| Antimony trioxide | $\text{Sb}_2\text{O}_3$       | 0.07287   |
| Arsenic           | $\text{As}$                   | 0.037461  |
| Arsenic pentoxide | $\text{As}_2\text{O}_5$       | 0.057460  |
| Arsenic trioxide  | $\text{As}_2\text{O}_3$       | 0.049460  |
| Arsenite          | $\text{AsO}_3$                | 0.061460  |
| Bleaching powder  | $\text{CaOCl}_2$              | 0.063493  |
| Bromine           | $\text{Br}$                   | 0.079909  |
| Chlorine          | $\text{Cl}$                   | 0.035453  |
| Chromic oxide     | $\text{Cr}_2\text{O}_3$       | 0.02533   |

**TABLE 11.28** Titrimetric (Volumetric) Factors (*Continued*)

| Iodine ( <i>continued</i> ) |                                                              |           |
|-----------------------------|--------------------------------------------------------------|-----------|
| Substance                   | Formula                                                      | Grams     |
| Chromium trioxide           | $\text{CrO}_3$                                               | 0.033331  |
| Copper                      | $\text{Cu}$                                                  | 0.06354   |
| Copper oxide                | $\text{CuO}$                                                 | 0.07954   |
| Copper sulfate              | $\text{CuSO}_4$                                              | 0.15960   |
| Copper sulfate              | $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$                    | 0.24968   |
| Ferric iron                 | $\text{Fe}^{3+}$                                             | 0.05585   |
| Ferric oxide                | $\text{Fe}_2\text{O}_3$                                      | 0.07985   |
| Hydrogen sulfide            | $\text{H}_2\text{S}$                                         | 0.017040  |
| Iodine                      | $\text{I}$                                                   | 0.126904  |
| Lead chromate               | $\text{PbCrO}_4$                                             | 0.10773   |
| Lead dioxide                | $\text{PbO}_2$                                               | 0.11959   |
| Nitrous acid                | $\text{HNO}_2$                                               | 0.023507  |
| Oxygen                      | $\text{O}$                                                   | 0.0079997 |
| Potassium chlorate          | $\text{KClO}_3$                                              | 0.020426  |
| Potassium chromate          | $\text{K}_2\text{CrO}_4$                                     | 0.064733  |
| Potassium dichromate        | $\text{K}_2\text{Cr}_2\text{O}_7$                            | 0.049032  |
| Potassium nitrite           | $\text{KNO}_2$                                               | 0.042554  |
| Potassium permanganate      | $\text{KMnO}_4$                                              | 0.031608  |
| Red lead                    | $\text{Pb}_3\text{O}_4$                                      | 0.34278   |
| Sodium chromate             | $\text{Na}_2\text{CrO}_4$                                    | 0.053991  |
| Sodium dichromate           | $\text{Na}_2\text{Cr}_2\text{O}_7$                           | 0.043661  |
| Sodium dichromate           | $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ | 0.049666  |
| Sodium nitrite              | $\text{NaNO}_2$                                              | 0.034498  |
| Sodium sulfide              | $\text{Na}_2\text{S}$                                        | 0.039022  |
| Sodium sulfide              | $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$              | 0.12009   |
| Sodium sulfite              | $\text{Na}_2\text{SO}_3$                                     | 0.063021  |
| Sodium sulfite              | $\text{Na}_2\text{SO}_3 \cdot 7\text{H}_2\text{O}$           | 0.12607   |
| Sodium thiosulfate          | $\text{Na}_2\text{S}_2\text{O}_3$                            | 0.15811   |
| Sulfur                      | $\text{S}$                                                   | 0.016032  |
| Sulfur dioxide              | $\text{SO}_2$                                                | 0.032031  |
| Sulfurous acid              | $\text{H}_2\text{SO}_3$                                      | 0.041039  |
| Tin                         | $\text{Sn}$                                                  | 0.059345  |

## Potassium dichromate

The following factors are the equivalent of 1 mL of *normal potassium dichromate*. Where the normality of the solution being used is other than normal, multiply the factors given in the table below by the normality of the solution employed.

| Substance            | Formula                                   | Grams     |
|----------------------|-------------------------------------------|-----------|
| Chromic oxide        | $\text{Cr}_2\text{O}_3$                   | 0.025332  |
| Chromium trioxide    | $\text{CrO}_3$                            | 0.033331  |
| Ferrous iron         | $\text{Fe}^{2+}$                          | 0.055847  |
| Ferrous oxide        | $\text{FeO}$                              | 0.071846  |
| Ferroso-ferric oxide | $\text{Fe}_3\text{O}_4$                   | 0.077180  |
| Ferrous sulfate      | $\text{FeSO}_4$                           | 0.15191   |
| Ferrous sulfate      | $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ | 0.27802   |
| Glycerol             | $\text{C}_3\text{H}_5(\text{OH})_3$       | 0.0065782 |
| Lead chromate        | $\text{PbCrO}_4$                          | 0.10773   |
| Zinc                 | $\text{Zn}$                               | 0.032685  |

**TABLE 11.28** Titrimetric (Volumetric) Factors (*Continued*)

## Potassium permanganate

The following factors are the equivalent of 1 mL of *normal potassium permanganate*. Where the normality of the solution being used is other than normal, multiply the factors given in the table below by the normality of the solution employed.

| Substance                                                             | Formula                                                             | Grams     |
|-----------------------------------------------------------------------|---------------------------------------------------------------------|-----------|
| Ammonium oxalate                                                      | $(\text{NH}_4)_2\text{C}_2\text{O}_4$                               | 0.062049  |
| Ammonium oxalate                                                      | $(\text{NH}_4)_2\text{C}_2\text{O}_4 \cdot \text{H}_2\text{O}$      | 0.071056  |
| Ammonium peroxydisulfate                                              | $(\text{NH}_4)_2\text{S}_2\text{O}_8$                               | 0.11410   |
| Antimony                                                              | Sb                                                                  | 0.060875  |
| Barium peroxide                                                       | $\text{BaO}_2$                                                      | 0.084669  |
| Barium peroxide                                                       | $\text{BaO}_2 \cdot 8\text{H}_2\text{O}$                            | 0.15673   |
| Calcium carbonate                                                     | $\text{CaCO}_3$                                                     | 0.050045  |
| Calcium oxide                                                         | CaO                                                                 | 0.02804   |
| Calcium peroxide                                                      | $\text{CaO}_2$                                                      | 0.036039  |
| Calcium sulfate                                                       | $\text{CaSO}_4$                                                     | 0.068071  |
| Calcium sulfate                                                       | $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$                           | 0.086086  |
| Ferric oxide                                                          | $\text{Fe}_2\text{O}_3$                                             | 0.079846  |
| Ferroso-ferric oxide                                                  | $\text{Fe}_3\text{O}_4$                                             | 0.077180  |
| Ferrous ammonium sulfate                                              | $\text{Fe}(\text{NH}_4)_2(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 0.39214   |
| Ferrous oxide                                                         | FeO                                                                 | 0.071846  |
| Ferrous sulfate                                                       | $\text{FeSO}_4$                                                     | 0.15191   |
| Ferrous sulfate                                                       | $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$                           | 0.27802   |
| Formic acid                                                           | $\text{HCO}_2\text{H}$                                              | 0.023013  |
| Hydrogen peroxide                                                     | $\text{H}_2\text{O}_2$                                              | 0.017007  |
| Iodine                                                                | I                                                                   | 0.126904  |
| Iron                                                                  | Fe                                                                  | 0.055847  |
| Manganese                                                             | Mn                                                                  | 0.010988  |
| Manganese dioxide                                                     | $\text{MnO}_2$                                                      | 0.043468  |
| Manganous oxide (Volhard)                                             | MnO                                                                 | 0.035469  |
| Molybdenum trioxide titration from yellow ppt.<br>after reduction     | $\text{MoO}_3$                                                      | 0.047979  |
| Oxalic acid                                                           | $(\text{CO}_2\text{H})_2$                                           | 0.045018  |
| Oxalic acid                                                           | $(\text{CO}_2\text{H})_2 \cdot 2\text{H}_2\text{O}$                 | 0.063033  |
| Phosphorus titration from yellow ppt. after reduction                 | P                                                                   | 0.0008604 |
| Phosphorus pentoxide to titration from yellow ppt.<br>after reduction | $\text{P}_2\text{O}_5$                                              | 0.0019715 |
| Potassium dichromate                                                  | $\text{K}_2\text{Cr}_2\text{O}_7$                                   | 0.049032  |
| Potassium nitrite                                                     | $\text{KNO}_2$                                                      | 0.042552  |
| Potassium persulfate                                                  | $\text{K}_2\text{S}_2\text{O}_8$                                    | 0.13516   |
| Sodium nitrite                                                        | $\text{NaNO}_2$                                                     | 0.034498  |
| Sodium oxalate                                                        | $\text{Na}_2\text{C}_2\text{O}_4$                                   | 0.067000  |
| Sodium persulfate                                                     | $\text{Na}_2\text{S}_2\text{O}_8$                                   | 0.11905   |
| Tin                                                                   | Sn                                                                  | 0.059345  |

**TABLE 11.28** Titrimetric (Volumetric) Factors (*Continued*)

## Silver nitrate

The following factors are the equivalent of 1 mL of *normal silver nitrate*. Where the normality of the solution being used is other than normal, multiply the factors given in the table below by the normality of the solution employed.

| Substance             | Formula                               | Grams    |
|-----------------------|---------------------------------------|----------|
| Ammonium bromide      | NH <sub>4</sub> Br                    | 0.097948 |
| Ammonium chloride     | NH <sub>4</sub> Cl                    | 0.053492 |
| Ammonium iodide       | NH <sub>4</sub> I                     | 0.14494  |
| Ammonium thiocyanate  | NH <sub>4</sub> SCN                   | 0.076120 |
| Barium chloride       | BaCl <sub>2</sub>                     | 0.10412  |
| Barium chloride       | BaCl <sub>2</sub> · 2H <sub>2</sub> O | 0.12214  |
| Bromine               | Br                                    | 0.079909 |
| Cadmium chloride      | CdCl <sub>2</sub>                     | 0.091653 |
| Cadmium iodide        | CdI <sub>2</sub>                      | 0.18310  |
| Calcium chloride      | CaCl <sub>2</sub>                     | 0.055493 |
| Chlorine              | Cl                                    | 0.035453 |
| Ferric chloride       | FeCl <sub>3</sub>                     | 0.054069 |
| Ferrous chloride      | FeCl <sub>2</sub>                     | 0.063377 |
| Hydriodic acid        | HI                                    | 0.12791  |
| Hydrobromic acid      | HBr                                   | 0.080917 |
| Hydrochloric acid     | HCl                                   | 0.036461 |
| Iodine                | I                                     | 0.126904 |
| Lithium chloride      | LiCl                                  | 0.042392 |
| Lead chloride         | PbCl <sub>2</sub>                     | 0.13905  |
| Magnesium chloride    | MgCl <sub>2</sub>                     | 0.047609 |
| Magnesium chloride    | MgCl <sub>2</sub> · 6H <sub>2</sub> O | 0.10166  |
| Potassium bromide     | KBr                                   | 0.11901  |
| Potassium chloride    | KCl                                   | 0.074555 |
| Potassium iodide      | KI                                    | 0.16601  |
| Potassium oxide       | K <sub>2</sub> O                      | 0.047102 |
| Potassium thiocyanate | KSCN                                  | 0.097184 |
| Silver                | Ag                                    | 0.10787  |
| Silver iodide         | AgI                                   | 0.23477  |
| Silver nitrate        | AgNO <sub>3</sub>                     | 0.16987  |
| Sodium bromide        | NaBr                                  | 0.10290  |
| Sodium bromide        | NaBr · 2H <sub>2</sub> O              | 0.13893  |
| Sodium chloride       | NaCl                                  | 0.058443 |
| Sodium iodide         | NaI                                   | 0.14989  |
| Sodium iodide         | NaI · 2H <sub>2</sub> O               | 0.18592  |
| Sodium oxide          | Na <sub>2</sub> O                     | 0.030990 |
| Strontium chloride    | SrCl <sub>2</sub>                     | 0.079263 |
| Strontium chloride    | SrCl <sub>2</sub> · 6H <sub>2</sub> O | 0.13331  |
| Zinc chloride         | ZnCl <sub>2</sub>                     | 0.068138 |

**TABLE 11.28** Titrimetric (Volumetric) Factors (*Continued*)

| Sodium thiosulfate   |                                                              |           |
|----------------------|--------------------------------------------------------------|-----------|
| Substance            | Formula                                                      | Grams     |
| Acetone              | $(\text{CH}_3)_2\text{CO}$                                   | 0.0096801 |
| Ammonium chromate    | $(\text{NH}_4)_2\text{CrO}_4$                                | 0.050690  |
| Antimony             | Sb                                                           | 0.06088   |
| Antimony trioxide    | $\text{Sb}_2\text{O}_3$                                      | 0.07287   |
| Bleaching powder     | $\text{CaOCl}_2$                                             | 0.063493  |
| Bromine              | Br                                                           | 0.079909  |
| Chlorine             | Cl                                                           | 0.035453  |
| Chromic oxide        | $\text{Cr}_2\text{O}_3$                                      | 0.02533   |
| Chromium trioxide    | $\text{CrO}_3$                                               | 0.033331  |
| Copper               | Cu                                                           | 0.06354   |
| Copper oxide         | CuO                                                          | 0.07954   |
| Copper sulfate       | $\text{CuSO}_4$                                              | 0.15960   |
| Copper sulfate       | $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$                    | 0.24968   |
| Iodine               | I                                                            | 0.126904  |
| Lead chromate        | $\text{PbCrO}_4$                                             | 0.10773   |
| Lead dioxide         | $\text{PbO}_2$                                               | 0.11959   |
| Nitrous acid         | $\text{HNO}_2$                                               | 0.023507  |
| Potassium chromate   | $\text{K}_2\text{CrO}_4$                                     | 0.064733  |
| Potassium dichromate | $\text{K}_2\text{Cr}_2\text{O}_7$                            | 0.049032  |
| Red lead             | $\text{Pb}_3\text{O}_4$                                      | 0.34278   |
| Sodium chromate      | $\text{Na}_2\text{CrO}_4$                                    | 0.053991  |
| Sodium dichromate    | $\text{Na}_2\text{Cr}_2\text{O}_7$                           | 0.043661  |
| Sodium dichromate    | $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ | 0.049666  |
| Sodium nitrite       | $\text{NaNO}_2$                                              | 0.034498  |
| Sodium thiosulfate   | $\text{Na}_2\text{S}_2\text{O}_3$                            | 0.15811   |
| Sodium thiosulfate   | $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$  | 0.24818   |
| Sulfur               | S                                                            | 0.016032  |
| Sulfur dioxide       | $\text{SO}_2$                                                | 0.032031  |
| Tin                  | Sn                                                           | 0.059345  |

**11.6.2 Titrimetric (Volumetric) Factors for Acid-Base Titrations**

Titrimetric (volumetric) factors for acids and bases are given in Table 11.28. Suitable indicators for acid-base titrations may be found in Tables 8.23 and 8.24.

**11.6.3 Standard Volumetric (Titrimetric) Redox Solutions**

**Alkaline arsenite**, 0.1*N* As(III) to As(V). Dissolve 4.9460 g of primary standard grade  $\text{As}_2\text{O}_3$  in 40 mL of 30% NaOH solution. Dilute with 200 mL of water. Acidify the solution with 6*N* HCl to the acid color of methyl red indicator. Add to this solution 40 g of  $\text{NaHCO}_3$  and dilute to 1 L.

**Ceric sulfate**, 0.1*N* Ce(IV) to Ce(III). Dissolve 63.26 g of cerium(IV) ammonium sulfate dihydrate in 500 mL of 2*N* sulfuric acid. Dilute the solution to 1 L and standardize against the

alkaline arsenite solution as follows: measure, accurately, 30 to 40 mL of arsenite solution into an Erlenmeyer flask and dilute to 150 mL. Add slowly, to prevent excessive frothing, 20 mL of 4*N* sulfuric acid, 2 drops of 0.01*M* osmium tetroxide solution, and 4 drops of 1,10-phenanthroline iron(II) complex indicator. Titrate with the ceric sulfate solution to a faint blue endpoint. Compute the normality of the ceric solution from the normality of the arsenite solution.

**Iron(II) ammonium sulfate hexahydrate**, 0.1*N* Fe(II) to Fe(III). Dissolve 39.2139 g of  $\text{FeSO}_4 \cdot 2(\text{NH}_4)_2\text{SO}_4 \cdot 6\text{H}_2\text{O}$  in 500 mL of 1*N* sulfuric acid and dilute to 1 L. If desired, check against standard dichromate or permanganate solution.

**Iodine**, 0.1*N* (0 to 1–). Dissolve 12.690 g of resublimed iodine in 25 mL of a solution containing 15 g of KI which is free from iodate. After all the solid has dissolved, dilute to 1 L. If desired, check against a standard arsenite or standard thiosulfate solution.

**Potassium bromate**, 0.1*N* (5+ to 1–). Weigh out 2.7833 g of  $\text{KBrO}_3$ , dissolve in water, and dilute to 1 L.

**Potassium dichromate**, 0.1*N* Cr(VI) to Cr(III). Weigh out 4.9030 g of  $\text{K}_2\text{Cr}_2\text{O}_7$  that has been dried at 120°C, dissolve in water, and dilute to 1 L.

**Potassium iodate**, 0.1*N* (5+ to 1–). Weigh out exactly 3.5667 g of  $\text{KIO}_3$  (free from iodide), dried at 120°C, and dissolve in water containing about 15 g of KI, and dilute to 1 L.

**Potassium permanganate**, 0.1*N* (7+ to 2+). Dissolve about 3.3 g in a liter of distilled water. Allow this to stand for 2 or 3 days, then siphon it carefully through clean glass tubes or filter it through a Gooch crucible into the glass container in which it is to be kept, discarding the first 25 mL and allowing the last inch of liquid to remain in the bottle. In this way any dust or reducing substance in the water is oxidized, and the  $\text{MnO}_2$  formed is removed. Permanganate solutions should never be allowed to come into contact with rubber, filter paper, or any other organic matter, and should be stored away from light. To standardize the  $\text{KMnO}_4$ , weigh accurately samples of about 0.3 g of primary standard grade  $\text{Na}_2\text{C}_2\text{O}_4$  into Erlenmeyer flasks, add 150 mL of distilled water and 4 mL of concentrated  $\text{H}_2\text{SO}_4$ , and heat to 70°C and maintain at this temperature throughout the titration with the permanganate solution. The end point is a faint, permanent pink color throughout the solution. Equivalent weight of  $\text{Na}_2\text{C}_2\text{O}_4/2$  is 67.000 g.

**Sodium thiosulfate**, 0.1*N*. Weigh 24.818 g of fresh crystals of  $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ , dissolve in distilled water. Add 0.5 g of  $\text{Na}_2\text{CO}_3$  and 0.5 mL of chloroform as preservative. Dilute to 1 L.

Equations for the principal methods for the redox determinations of the elements are given in Table 11.29. Volumetric factors in redox titrations for the common titrants are given in Table 11.28.

### 11.6.4 Indicators for Redox Titrations

A selected list of redox indicators will be found in Table 8.26. A redox indicator should be selected so that its  $E^0$  is approximately equal to the electrode potential at the equivalent point, or so that the color change will occur at an appropriate part of the titration curve. If  $n$  is the number of electrons involved in the transition from the reduced to the oxidized form of the indicator, the range in which the color change occurs is approximately given by  $E^0 \pm 0.06/n$  volt (V) for a two-color indicator whose forms are equally intensely colored. Since hydrogen ions are involved in the redox equilibria of many indicators, it must be recognized that the color change interval of such an indicator will vary with pH.

In Table 8.26,  $E^0$  represents the redox potential at which the color change of the indicator would normally be perceived in a solution containing approximately  $1\text{M H}^+$ . For a one-color indicator this is the potential at which the concentration of the colored form is just large enough to impart a visible color to the solution and depends on the total concentration of indicator added to the solution. If it is the reduced form of the indicator that is colorless, the potential at which the first visible color

appears becomes less positive as the total concentration of indicator increases. For a two-color indicator, the potential at which the middle tint appears is independent of the total indicator concentration, but may differ from the potentiometrically determined formal potential of the indicator in either direction, depending on which of the two forms is more intensely colored. If the reduced form is the more intense color, the middle tint will appear at a potential more positive than the potentiometrically measured formal potential, which is the potential at which the two forms are present at equal concentrations.

In addition to those indicators listed in Table 8.26, there are indicators for bromometric and iodometric titrations:

*Specific reagents for titrations with bromine or bromate*

|                             |                                                                                                   |
|-----------------------------|---------------------------------------------------------------------------------------------------|
| Methyl orange or methyl red | Use acid-base indicator solutions. Oxidation causes bleaching of indicator to colorless           |
| Bordeaux acid red 17        | Dissolve 2 g dye in 1 L water. The red solution is oxidized to pale yellowish green or colorless. |
| Naphthol blue black         | Dissolve 2 g dye in 1 L water. The blue solution is oxidized to pale red.                         |

*Specific reagents for iodometric titrations*

|                                                           |                                                                                                                                                                                                                                        |
|-----------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Organic solvents such as $\text{CCl}_4$ , $\text{CHCl}_3$ | Up to 5 mL solvent is usually added per titration. Near the end point the mixture is shaken vigorously after each addition of titrant, and the appearance or disappearance of the $\text{I}_2$ color in the organic layer is observed. |
| Starch                                                    | Suspend 5 g of soluble starch in 50 mL of saturated NaCl solution, and stir slowly into 500 mL of boiling saturated NaCl solution. Cool and bottle. Free iodine produces a blue-black color.                                           |

**TABLE 11.29** Equations for the Redox Determinations of the Elements with Equivalent Weights

|                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Al              | $\text{Al}(\text{C}_6\text{H}_5\text{NO})_3 + 3 \text{HCl} = \text{AlCl}_3 + 3 \text{C}_6\text{H}_7\text{NO}$ (8-hydroxyquinoline)<br>$3 \text{C}_6\text{H}_7\text{NO} + 6 \text{Br}_2 = 3 \text{C}_6\text{H}_5\text{Br}_2\text{NO} + 6 \text{HBr}$<br>$\text{Al}/12 = 2.2485; \text{Al}_2\text{O}_3/24 = 4.2483$                                                                                                                                                                                                                                                                                                                                 |
| As <sup>0</sup> | $\text{As} + 5 \text{Ce(IV)} + 4 \text{H}_2\text{O} = \text{H}_3\text{AsO}_4 + 5 \text{Ce(III)} + 5 \text{H}^+$<br>$\text{As}/5 = 14.9843$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| As(III)         | $5 \text{H}_3\text{AsO}_3 + 2 \text{KMnO}_4 + 6 \text{HCl} = 5 \text{H}_3\text{AsO}_4 + 2 \text{MnCl}_2 + 3 \text{H}_2\text{O}$<br>$\text{H}_3\text{AsO}_3 + 2 \text{Ce}(\text{SO}_4)_2 + \text{H}_2\text{O} = \text{H}_3\text{AsO}_4 + \text{Ce}_2(\text{SO}_4)_3 + \text{H}_2\text{SO}_4$<br>$\text{As}/2 = 37.4608; \text{As}_2\text{O}_3/4 = 49.460$<br>$3 \text{H}_3\text{AsO}_3 + \text{KBrO}_3 (+ \text{HCl}) = 3 \text{H}_3\text{AsO}_4 + \text{KBr}$<br>$\text{H}_3\text{AsO}_3 + \text{I}_2 + 2 \text{H}_2\text{O} = \text{H}_3\text{AsO}_4 + 2 \text{I}^- + 2 \text{H}^+$<br>$\text{As}/2 = 37.4608; \text{As}_2\text{O}_3/4 = 49.460$ |
| As(V)           | $\text{H}_3\text{AsO}_4 + 2 \text{KI} (\text{excess}) + 2 \text{HCl} = \text{H}_3\text{AsO}_3 + \text{I}_2 + 2 \text{KCl} + \text{H}_2\text{O}$<br>$\text{I}_2 + 2 \text{Na}_2\text{S}_2\text{O}_3 = 2 \text{NaI} + \text{Na}_2\text{S}_4\text{O}_6$<br>$\text{As}/2 = 37.4608; \text{As}_2\text{O}_3/4 = 49.460$                                                                                                                                                                                                                                                                                                                                 |

**TABLE 11.29** Equations for the Redox Determinations of the Elements with Equivalent Weights (*Continued*)

|                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|-----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ba                          | $\text{BaCrO}_4 + 6 \text{ KI (excess)} + 16 \text{ HCl} = 2 \text{ BaCl}_2 + 3 \text{ I}_2 + 6 \text{ KCl} + 2 \text{ CrCl}_3 + 8 \text{ H}_2\text{O}$ $\text{I}_2 + 2 \text{ Na}_2\text{S}_2\text{O}_3 = 2 \text{ NaI} + \text{Na}_2\text{S}_4\text{O}_6 \quad \text{Ba/3} = 45.78$ $\text{BaCrO}_4 + 3 \text{ Fe}^{2+} \text{ (excess)} + 8 \text{ H}^+ = \text{Ba}^{2+} + \text{Cr}^{3+} + 3 \text{ Fe}^{3+} + 4 \text{ H}_2\text{O}$ Titrate excess $\text{Fe}^{2+}$ with permanganate or dichromate; $\text{Ba/3} = 45.78$                                                                                                               |
| $\text{Br}_2$               | $\text{Br}_2 + 2 \text{ KI (excess)} = 2 \text{ KBr} + \text{I}_2$ $\text{I}_2 + 2 \text{ Na}_2\text{S}_2\text{O}_3 \rightarrow 2 \text{ NaI} + \text{Na}_2\text{S}_4\text{O}_6 \quad \text{Br}_2/2 = 79.904$                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| $\text{Br}^-$               | $\text{Br}^- + 3 \text{ HClO} = \text{BrO}_3^- + 3 \text{ Cl}^- + 3 \text{ H}^+$ $\text{Br/6} = 13.317$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| $\text{BrO}_3^-$            | $\text{BrO}_3^- + 6 \text{ I}^- \text{ (excess)} + 6 \text{ H}^+ = \text{Br}^- + 3 \text{ I}_2 + 3 \text{ H}_2\text{O}$ $\text{I}_2 + 2 \text{ Na}_2\text{S}_2\text{O}_3 = 2 \text{ NaI} + \text{Na}_2\text{S}_4\text{O}_6$ $\text{KBrO}_3/6 = 27.835$                                                                                                                                                                                                                                                                                                                                                                                         |
| CO                          | $5 \text{ CO} + \text{I}_2\text{O}_5 = 5 \text{ CO}_2 + \text{I}_2 \text{ (at } 125^\circ\text{C; adsorbed and measured colorimetrically)}$ $5/2 \text{ CO} = 70.02$                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| $\text{C}_2\text{O}_4^{2-}$ | Titrate as for $\text{CaC}_2\text{O}_4$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| $\text{C}_2\text{O}_6^{2-}$ | Acidify and titrate as for $\text{H}_2\text{O}_2$ ; $\text{C}_2\text{O}_6^{2-} + 2 \text{ H}^+ = \text{H}_2\text{O}_2 + \text{CO}_2$<br>$\text{K}_2\text{C}_2\text{O}_6/2 = 99.11$                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Ca                          | $5 \text{ CaC}_2\text{O}_4 + 2 \text{ KMnO}_4 + 8 \text{ H}_2\text{SO}_4 = 5 \text{ CaSO}_4 + 10 \text{ CO}_2 + \text{K}_2\text{SO}_4 + 2 \text{ MnSO}_4 + 8 \text{ H}_2\text{O}$ $\text{Ca/2} = 20.039; \text{CaO/2} = 28.04$                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Cd                          | $\text{Cd(anthranilate)}_2 + 4 \text{ Br}_2 = 2 \text{ NH}_2\text{C}_6\text{H}_2\text{Br}_2\text{COOH} + 4 \text{ Br}^-$ Titrate with $\text{KBrO}_3$ — $\text{KBr}$ until color of indigo changes to yellow.<br>Add $\text{KI}$ and back-titrate iodine liberated with thiosulfate. $\text{Cd/8} = 14.05$                                                                                                                                                                                                                                                                                                                                     |
| Ce                          | Oxidize $\text{Ce(III)}$ to $\text{Ce(IV)}$ with $(\text{NH}_4)_2\text{S}_2\text{O}_8$ plus $\text{Ag}^+$ ; destroy excess by boiling.<br>$2 \text{ Ce(SO}_4)_2 + 2 \text{ FeSO}_4 = \text{Ce}_2(\text{SO}_4)_3 + \text{Fe}_2(\text{SO}_4)_3$ $\text{Ce/1} = 140.12; \text{Ce}_2\text{O}_3/2 = 164.12$                                                                                                                                                                                                                                                                                                                                         |
| $\text{Cl}_2$               | Same as for $\text{Br}_2$ ; $\text{Cl}_2/2 = 35.453$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| $\text{ClO}^-$              | $\text{ClO}^- + 2 \text{ I}^- + 2 \text{ H} = \text{Cl}^- + \text{I}_2 + \text{H}_2\text{O}$ Titrate liberated $\text{I}_2$ with thiosulfate; $\text{HClO/2} = 26.230$                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| $\text{ClO}_2^-$            | $\text{ClO}_2^- + 4 \text{ I}^- + 4 \text{ H}^+ = \text{Cl}^- + 2 \text{ I}_2 + 2 \text{ H}_2\text{O}$ Titrate liberated $\text{I}_2$ with thiosulfate; $\text{HClO/2} = 26.230$                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| $\text{ClO}_3^-$            | $\text{ClO}_3^- + 6 \text{ I}^- + 6 \text{ H}_2\text{O} = \text{Cl}^- + 3 \text{ I}_2 + 3 \text{ H}_2\text{O}$ Titrated liberated $\text{I}_2$ with thiosulfate; $\text{HClO}_2/4 = 17.115$<br>$\text{ClO}_3^- + 3 \text{ H}_3\text{AsO}_3 \text{ (excess; boil with strong HCl)} = \text{Cl}^- + 3 \text{ H}_3\text{AsO}_4$ Titrate excess $\text{H}_3\text{AsO}_3$ with bromate; $\text{HClO}_3/6 = 14.077$                                                                                                                                                                                                                                  |
| Co                          | $\text{Co(NH}_3)_6^{3+} + \text{Fe(CN)}_6^{3-} \text{ [Citrate-NH}_3 \text{ buffer]} = \text{Co(NH}_3)_6^{3+} + \text{Fe(CN)}_6^{4-}$ $\text{Co/1} = 58.9332$ Precipitate $\text{Co}$ anthranilate and treat as for cadmium; $\text{Co/8} = 7.3667$                                                                                                                                                                                                                                                                                                                                                                                            |
| Cr                          | $\text{Cr}_2\text{O}_7^{2-} + 6 \text{ Fe}^{2+} + 14 \text{ H}^+ = 2 \text{ Cr}^{3+} + 6 \text{ Fe}^{3+} + 7 \text{ H}_2\text{O}$ $\text{Cr/3} = 17.332; \text{Cr}_2\text{O}_3/6 = 25.337$                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| Cu                          | $2 \text{ Cu}^{2+} + 2 \text{ I}^- + 2 \text{ SCN}^- = 2 \text{ CuSCN} + \text{I}_2$ Titrate the liberated iodine with thiosulfate; $\text{Cu/1} = 63.546$<br>$4 \text{ CuSCN} + 7 \text{ IO}_3^- + 14 \text{ H}^+ + 7 \text{ Cl}^- = 4 \text{ Cu}^{2+} + 4 \text{ SO}_4^{2-} + 7 \text{ ICl} + 4 \text{ HCN} + 5 \text{ H}_2\text{O}$ Precipitate and wash $\text{CuSCN}$ . Titrate with standard $\text{KIO}_3$ solution with 5 mL $\text{CHCl}_3$ until a definite $\text{I}_2$ color appears in the organic layer. Back-titrate the excess $\text{I}_2$ with standard thiosulfate solution. $\text{Cu/7} = 9.078; \text{KIO}_3/4 = 53.505$ |
| $\text{Fe(II)}$             | $5 \text{ Fe}^{2+} + \text{MnO}_4^- + 8 \text{ H}^+ = 5 \text{ Fe}^{3+} + \text{Mn}^{2+} + 4 \text{ H}_2\text{O}$ $\text{Fe}^{2+} + \text{Ce(IV)} = \text{Fe}^{3+} + \text{Ce(III)}; \text{ use 1,10-phenanthroline iron(II) indicator.}$ $6 \text{ Fe}^{2+} + \text{Cr}_2\text{O}_7^{2-} + 14 \text{ H}^+ = 6 \text{ Fe}^{3+} + 2 \text{ Cr}^{3+} + 7 \text{ H}_2\text{O}; \text{ use diphenylamine sulfonate indicator.}$ $\text{Fe/1} = 55.847; \text{Fe}_2\text{O}_3/2 = 79.845$                                                                                                                                                           |



**TABLE 11.29** Equations for the Redox Determinations of the Elements with Equivalent Weights (*Continued*)

|                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Fe(III)                | $\text{Fe}^{3+} + 4 \text{SCN}^- = \text{Fe}(\text{SCN})_4^-; \text{Fe}(\text{SCN})_4^- + \text{Ti(III)} = \text{Fe}^{2+} + \text{Ti(IV)} + 4 \text{SCN}^-$ $\text{Fe/1} = 55.847; \text{Fe}_2\text{O}_3/2 = 79.845$ $2 \text{Fe}^{3+} + \text{Zn} = 2 \text{Fe}^{2+} + \text{Zn}^{2+}; \text{then proceed by a method under Fe(II).}$ $\text{Fe}^{3+} + \text{Ag} + \text{Cl}^- = \text{Fe}^{2+} + \text{AgCl}; \text{then proceed by a method under Fe(II).}$ $2 \text{Fe}^{3+} + \text{SnCl}_2(\text{slight excess}) + 4 \text{Cl}^- = 2 \text{Fe}^{2+} + \text{SnCl}_6^{2-}$ $2 \text{HgCl}_2 + \text{SnCl}_2 + 2 \text{Cl}^- = \text{Hg}_2\text{Cl}_2 + \text{SnCl}_6^{2-}$ <p>Pour above mixture into an <math>\text{H}_3\text{PO}_4</math> plus <math>\text{MnSO}_4</math> solution and titrate with <math>\text{KMnO}_4</math> as under Fe(II).</p> $\text{Fe/1} = 55.847; \text{Fe}_2\text{O}_3/2 = 79.845$ $2 \text{Fe}^{3+} + 2 \text{I}^- = \text{Fe}^{2+} + \text{I}_2$ <p>Titrate liberated iodine with thiosulfate; <math>\text{Fe/1} = 55.847; \text{Fe}_2\text{O}_3/2 = 79.845</math></p>                                                                        |
| $\text{I}_2$           | $\text{I}_2 + 2 \text{S}_2\text{O}_3^{2-} = 2 \text{I}^- + \text{S}_4\text{O}_6^{2-} \text{ [titrate solution (pH } \circ 7.0) \text{ with thiosulfate until color is pale yellow. Add KI and starch and continue titration to disappearance of blue color. } \text{I}_2/2 = 126.9045$ $\text{I}_2 + \text{H}_3\text{AsO}_3 + \text{H}_2\text{O} = 2 \text{I}^- + \text{H}_3\text{AsO}_4 + 2 \text{H}^+; \text{use starch and KI as indicator. } \text{I}_2/2 = 126.9045$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| $\text{I}^-$           | $2 \text{I}^- + \text{Br}_2(\text{excess}) = \text{I}_2 + 2\text{Br}^-$ <p>Remove excess <math>\text{Br}_2</math> formic acid and titrate <math>\text{I}_2</math> with thiosulfate. <math>\text{I}_2/2 = 126.9045</math></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| $\text{IO}_3^-$        | $\text{IO}_3^- + 5 \text{I}^- (\text{excess}) + 6 \text{H}^+ = 3 \text{I}_2 + 3 \text{H}_2\text{O}; \text{titrate } \text{I}_2 \text{ with thiosulfate. } \text{KIO}_3/6 = 35.67$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| $\text{IO}_4^-$        | $\text{IO}_4^- + 7 \text{I}^- (\text{excess}) + 8 \text{H}^+ = 4 \text{I}_2 + 4 \text{H}_2\text{O}; \text{use a neutral buffered solution. Titrate } \text{I}_2 \text{ with thiosulfate. } \text{KIO}_4/2 = 115.00$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| K                      | $\text{K}_2\text{Na}[\text{Co}(\text{NO}_2)_6]; \text{dissolve in } \text{H}_2\text{SO}_4 \text{ and titrate with either } \text{KMnO}_4 \text{ or } \text{Ce(IV)}. \text{ ca. } \text{K/5.5} \text{ but use an empirical factor.}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Mg                     | $\text{Mg}(\text{oxine})_2; \text{dissolve precipitate and use procedure for } \text{Al(8-hydroxyquinoline)}_3. \text{ Mg/8} = 3.0381$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Mn(II)                 | $2 \text{Mn}^{2+} + 5 \text{BiO}_3^- + 14 \text{H}^+ = 2 \text{MnO}_4^- + 5 \text{Bi}^{3+} + 7 \text{H}_2\text{O}$ $2 \text{MnO}_4^- + 5 \text{AsO}_3^{3-} + 6 \text{H}^+ = 2 \text{Mn}^{2+} + 5 \text{AsO}_4^{3-} + 3 \text{H}_2\text{O}; \text{Mn/5} = 10.9876$ $2 \text{Mn}^{2+} + 5 \text{S}_2\text{O}_8^{2-} + 8 \text{H}_2\text{O} (\text{Ag}^+ \text{ catalyst}) = 2 \text{MnO}_4^- + 10 \text{SO}_4^{2-} + 16 \text{H}^+$ <p>Titrate the permanganate formed with iron(II) as under iron(II); <math>\text{Mn/5} = 10.9876</math></p> $2 \text{Mn}^{2+} + 5 \text{IO}_4^- + 3 \text{H}_2\text{O} = 2 \text{MnO}_4^- + 5 \text{IO}_3^- + 6 \text{H}^+$ <p>Slowly precipitate excess <math>\text{KIO}_4</math> with <math>\text{Hg}(\text{NO}_3)_2</math>. Filter, add excess <math>\text{Fe}^{2+}</math> and titrate excess with standard <math>\text{KMnO}_4</math> solution; <math>\text{Mn/5} = 10.9876</math></p> $\text{MnO}_4^- + 4 \text{Mn}^{2+} + 15 \text{H}_2\text{P}_2\text{O}_7^- [\text{pH range 4 to 7}] = 5 \text{Mn}(\text{H}_2\text{P}_2\text{O}_7)_3^{3-} + 4 \text{H}_2\text{O}$ <p>Use Pt—SCE indicator system; <math>\text{Mn/1} = 54.9380</math></p> |
| Mn(IV)                 | $\text{MnO}_2 + 2 \text{Fe}^{2+}(\text{excess standard}) + 4 \text{H}^+ = \text{Mn}^{2+} + 2 \text{Fe}^{3+} + 2 \text{H}_2\text{O} (\text{use } \text{CO}_2 \text{ atmosphere})$ $\text{MnO}_2 + \text{H}_2\text{C}_2\text{O}_4(\text{excess standard}) + 2 \text{H}^+ = \text{Mn}^{2+} + 2 \text{CO}_2 + 2 \text{H}_2\text{O} (\text{use } \text{CO}_2 \text{ atmosphere})$ <p>In either of the above, titrate excess with <math>\text{KMnO}_4</math>. <math>\text{Mn/2} = 27.469; \text{MnO}_2/2 = 43.47</math></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Mn(VI)                 | $\text{MnO}_4^{2-} + 2 \text{H}_2\text{C}_2\text{O}_4 + 4 \text{H}^+ = \text{Mn}^{2+} + 4 \text{CO}_2 + 4 \text{H}_2\text{O} \text{ Add excess oxalate and back-titrate with permanganate. } \text{Mn/4} = 13.7345$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Mn(VII)                | $2 \text{MnO}_4^- + 5 \text{H}_2\text{C}_2\text{O}_4 + 6 \text{H}^+ = 2 \text{Mn}^{2+} + 10 \text{CO}_2 + 3 \text{H}_2\text{O}; \text{Mn/5} = 10.9876$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Mo                     | $\text{Mo(VI)} + \text{Zn} = \text{Mo(III)} + \text{Zn}^{2+}; \text{catch eluate in excess } \text{Fe}_2(\text{SO}_4)_3 \text{ solution}$ $\text{Mo(III)} + 3 \text{Fe}^{3+} + 4 \text{H}_2\text{O} = \text{MoO}_4^{2-} + 3 \text{Fe}^{2+} + 8 \text{H}^+; \text{titrate Fe(II) with } \text{KMnO}_4$ $\text{Mo/3} = 31.98$ $\text{Mo(VI)} + \text{Ag} + \text{Cl}^- = \text{Mo(V)} + \text{AgCl}; \text{pass through Ag reductor at } 60\text{--}80^\circ\text{C.}$ $\text{Mo(V)} + \text{Ce(IV)} = \text{Mo(VI)} + \text{Ce(III)}; \text{Mo/1} = 95.94$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| $\text{N}_2\text{H}_4$ | $3 \text{N}_2\text{H}_4 + 2 \text{BrO}_3^- (\text{excess}) = 3 \text{N}_2 + 2 \text{Br}^- + 6 \text{H}_2\text{O}; \text{add excess KI and titrate } \text{I}_2 \text{ with thio-sulfate. } \text{N}_2\text{H}_4/4 = 8.01$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| $\text{NH}_2\text{OH}$ | $\text{NH}_2\text{OH} + \text{BrO}_3^- = \text{NO}_3^- + \text{Br}^- + \text{H}^+ + \text{H}_2\text{O}; \text{proceed as above for } \text{N}_2\text{H}_4. \text{NH}_2\text{OH/6} = 5.505$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |

**TABLE 11.29** Equations for the Redox Determinations of the Elements with Equivalent Weights (*Continued*)

|                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| HN <sub>3</sub>                                 | 2 HN <sub>3</sub> + 2 Ce(IV)(excess) = 3 N <sub>2</sub> + 2 Ce(III) + 2 H <sup>+</sup> ; done under inert atmosphere.<br>Add excess KI and titrate with thiosulfate. HN <sub>3</sub> /1 = 43.03                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| NO <sub>2</sub> <sup>-</sup>                    | 5 NO <sub>2</sub> <sup>-</sup> + 2 MnO <sub>4</sub> <sup>-</sup> (excess) + 6 H <sup>+</sup> = 5 NO <sub>3</sub> <sup>-</sup> + 2 Mn <sup>2+</sup> + 3 H <sub>2</sub> O; determine excess KMnO <sub>4</sub><br>standard Na <sub>2</sub> C <sub>2</sub> O <sub>4</sub> solution. NaNO <sub>2</sub> /1 = 69.00<br>NO <sub>2</sub> <sup>-</sup> + 2 Ce(IV)(excess) + H <sub>2</sub> O = NO <sub>3</sub> <sup>-</sup> + 2 Ce(III) + 2 H <sup>+</sup> ; warmed to 50°C. Add excess<br>standard Fe(II) solution and back-titrate with standard Ce(IV) using erioglaucine indicator.<br>NaNO <sub>2</sub> /1 = 69.00                                                                                                                                                                                 |
| NO <sub>3</sub> <sup>-</sup>                    | NO <sub>3</sub> <sup>-</sup> + excess Fe <sup>2+</sup> (Mo catalyst) + 4 H <sup>+</sup> = NO + Fe <sup>3+</sup> . Add H <sub>3</sub> PO <sub>4</sub> and back-titrate excess<br>Fe(II) with K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> . NaNO <sub>3</sub> /3 = 28.34                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Nb(V)                                           | Nb(V) + Zn = Nb(III) + Zn <sup>2+</sup> ; catch reduced solution under excess Fe(III).<br>Nb(III) + 2 Fe <sup>3+</sup> = Nb(V) + 2 Fe <sup>2+</sup> ; titrate Fe(II) with MnO <sub>4</sub> solution using 1,10-phenanthro-<br>line as indicator. Nb/2 = 46.453; Nb <sub>2</sub> O <sub>5</sub> = 66.455                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Ni                                              | Precipitate Ni(anthranilate) <sub>2</sub> and proceed as under Cd. Ni/8 = 7.336                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| O <sub>2</sub>                                  | O <sub>2</sub> + 2 Mn <sup>2+</sup> + 2 OH <sup>-</sup> = 2 MnO <sub>2</sub> + 2 H <sup>+</sup> ; stoppered flask plus KI<br>MnO <sub>2</sub> + 2 I <sup>-</sup> + 4 H <sup>+</sup> = Mn <sup>2+</sup> + I <sub>2</sub> 2H <sub>2</sub> O; titrate I <sub>2</sub> released with thiosulfate. O <sub>2</sub> /4 =<br>7.007                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| O <sub>3</sub>                                  | O <sub>3</sub> + 2 I <sup>-</sup> + H <sub>2</sub> O = O <sub>2</sub> + I <sub>2</sub> + 2 OH <sup>-</sup> ; acidify and titrate with thiosulfate. O <sub>3</sub> /2 = 24.00                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| H <sub>2</sub> O <sub>2</sub>                   | 5 H <sub>2</sub> O <sub>2</sub> + 2 MnO <sub>4</sub> <sup>-</sup> + 6 H <sup>+</sup> = 5 O <sub>2</sub> + 2 Mn <sup>2+</sup> + 8 H <sub>2</sub> O; H <sub>2</sub> O <sub>2</sub> /2 = 17.01<br>H <sub>2</sub> O <sub>2</sub> + 2 Ce(IV) + 2 H <sup>+</sup> = 2 Ce(III) + 2 H <sub>2</sub> O; use 1,10-phenanthroline indicator<br>H <sub>2</sub> O <sub>2</sub> /1 = 34.02<br>H <sub>2</sub> O <sub>2</sub> + 2 I <sup>-</sup> + 2 H <sup>+</sup> = I <sub>2</sub> + 2 H <sub>2</sub> O; titrate I <sub>2</sub> with thiosulfate. H <sub>2</sub> O <sub>2</sub> /2 = 17.01<br>H <sub>2</sub> O <sub>2</sub> + 2 Ti(III) + 2 H <sup>+</sup> = 2 Ti(IV) + 2 H <sub>2</sub> O; end point is disappearance of the yellow color<br>of peroxotitanic acid. H <sub>2</sub> O <sub>2</sub> /2 = 17.01 |
| P                                               | The yellow precipitate of (NH <sub>4</sub> ) <sub>3</sub> [P(Mo <sub>3</sub> O <sub>10</sub> ) <sub>4</sub> ] is dissolved in NH <sub>4</sub> OH, then solution is strongly<br>acidified with H <sub>2</sub> SO <sub>4</sub> . See molybdenum; 12 moles Mo per P. P/36 = 0.86038                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| HPH <sub>2</sub> O <sub>2</sub>                 | HPH <sub>2</sub> O <sub>2</sub> + 2 I <sub>2</sub> (excess) + 2 H <sub>2</sub> O = H <sub>3</sub> PO <sub>4</sub> + 4 I <sup>-</sup> + 4 H <sup>+</sup> (let stand 10 h)<br>Make solution alkaline with NaHCO <sub>3</sub> and titrate excess I <sub>2</sub> with standard arsenite solution.<br>HPH <sub>2</sub> O <sub>2</sub> /4 = 16.499                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| H <sub>3</sub> PO <sub>3</sub>                  | H <sub>3</sub> PO <sub>3</sub> + I <sub>2</sub> (excess) + H <sub>2</sub> O = H <sub>3</sub> PO <sub>4</sub> + 2 I <sup>-</sup> + 2 H <sup>+</sup> (use CO <sub>2</sub> /NaHCO <sub>3</sub> buffer; let stand 40–<br>60 min in stoppered flask). Titrate excess I <sub>2</sub> with standard arsenite solution. H <sub>3</sub> PO <sub>3</sub> /2 =<br>41.00                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Pb                                              | Isolate Pb as PbSO <sub>4</sub> , dissolve it in NaOAc and precipitate with K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> . Dissolve K <sub>2</sub> CrO <sub>4</sub> in<br>NaCl—HCl solution, add KI, and titrate I <sub>2</sub> with thiosulfate solution.<br>2 PbCrO <sub>4</sub> + 6 I <sup>-</sup> + 16 H <sup>+</sup> = 2 Pb <sup>2+</sup> + 2 Cr <sup>3+</sup> + 3 I <sub>2</sub> + 8 H <sub>2</sub> O Pb/3 = 69.1; PbO/3 =<br>74.4                                                                                                                                                                                                                                                                                                                                                     |
| S <sup>2-</sup>                                 | H <sub>2</sub> S + I <sub>2</sub> (excess) = S + 2 I <sup>-</sup> + 2 H <sup>+</sup> Back-titrate excess I <sub>2</sub> with standard thiosulfate solution.<br>S/2 = 16.03; H <sub>2</sub> S/2 = 17.04<br>H <sub>2</sub> S + 4 Br <sub>2</sub> + 4 H <sub>2</sub> O = SO <sub>4</sub> <sup>2-</sup> + 8 Br <sup>-</sup> + 10 H <sup>+</sup> Use excess KBr and standard KBrO <sub>3</sub><br>solution. Let stand until clear, add excess KI, and titrate with standard thiosulfate solution.<br>H <sub>2</sub> S/8 = 4.260; SO <sub>2</sub> /2 = 32.03; SCN/6 = 9.681                                                                                                                                                                                                                         |
| SO <sub>2</sub> , SO <sub>3</sub> <sup>2-</sup> | SO <sub>2</sub> + I <sub>2</sub> + 2 H <sub>2</sub> O = SO <sub>4</sub> <sup>2-</sup> + 2 I <sup>-</sup> + 4 H <sup>+</sup> (Titrate excess I <sub>2</sub> with standard thiosulfate)<br>SO <sub>2</sub> /2 = 32.03<br>SO <sub>2</sub> + 4 Br <sub>2</sub> + 2 H <sub>2</sub> O = SO <sub>4</sub> <sup>2-</sup> + 2 Br <sup>-</sup> + 4 H <sup>+</sup> (Titrate with standard KBrO <sub>3</sub> —KBr solu-<br>tion until methyl orange is bleached.) SO <sub>2</sub> /2 = 32.03                                                                                                                                                                                                                                                                                                               |
| S <sub>2</sub> O <sub>3</sub> <sup>2-</sup>     | 2 S <sub>2</sub> O <sub>3</sub> <sup>2-</sup> + I <sub>2</sub> = S <sub>4</sub> O <sub>6</sub> <sup>2-</sup> + 2 I <sup>-</sup> (Use starch indicator) Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> /1 = 158.11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| H <sub>2</sub> SO <sub>5</sub>                  | SO <sub>5</sub> <sup>2-</sup> + H <sub>3</sub> AsO <sub>3</sub> = SO <sub>4</sub> <sup>2-</sup> + H <sub>3</sub> AsO <sub>4</sub> H <sub>2</sub> SO <sub>5</sub> /2 = 57.04                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| S <sub>2</sub> O <sub>8</sub> <sup>2-</sup>     | S <sub>2</sub> O <sub>8</sub> <sup>2-</sup> + H <sub>3</sub> AsO <sub>3</sub> + H <sub>2</sub> O = 2 SO <sub>4</sub> <sup>2-</sup> + H <sub>3</sub> AsO <sub>4</sub> + 2 H <sup>+</sup> H <sub>2</sub> S <sub>2</sub> O <sub>8</sub> /2 = 97.07<br>S <sub>2</sub> O <sub>8</sub> <sup>2-</sup> + 2 Fe <sup>2+</sup> = 2 SO <sub>4</sub> <sup>2-</sup> + 2 Fe <sup>3+</sup> H <sub>2</sub> S <sub>2</sub> O <sub>8</sub> /2 = 97.07                                                                                                                                                                                                                                                                                                                                                            |

**TABLE 11.29** Equations for the Redox Determinations of the Elements with Equivalent Weights (*Continued*)

|                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Sb                  | $5 \text{ Sb(III)} + 2 \text{ MnO}_4^- + 16 \text{ H}^+ = 5 \text{ Sb(V)} + 2 \text{ Mn}^{2+} + 8 \text{ H}_2\text{O}$<br>$3 \text{ Sb(III)} + \text{BrO}_3^- + 6 \text{ H}^+ = 3 \text{ Sb(V)} + \text{Br}^- + 3 \text{ H}_2\text{O}$<br>$\text{Sb(III)} + \text{I}_2 \text{ [tartrate buffer, pH >7]} = \text{Sb(V)} + 2 \text{ I}^-$<br>$\text{Sb(III)} + 2 \text{ Ce(IV)} = \text{Sb(V)} + 2 \text{ Ce(III)}$<br>For all four methods: $\text{Sb}/2 = 60.88$ ; $\text{Sb}_2\text{O}_3/4 = 72.88$                                                                                                                                                                                                                                                                                                                                                                                     |
| $\text{SeO}_3^{2-}$ | $5 \text{ H}_2\text{SeO}_3 + 2 \text{ MnO}_4^- + 6 \text{ H}^+ = 5 \text{ H}_2\text{SeO}_4 + 2 \text{ Mn}^{2+} + 3 \text{ H}_2\text{O}$ $\text{Na}_2\text{SeO}_3/2 = 86.47$<br>$\text{H}_2\text{SeO}_3 + 4 \text{ I}^- + 4 \text{ H}^+ = \text{Se} + 2 \text{ I}_2 + 3 \text{ H}_2\text{O}$ (titrate $\text{I}_2$ with standard thiosulfate solution)<br>$\text{Na}_2\text{SeO}_3/2 = 86.47$<br>$\text{H}_2\text{SeO}_3 + 4 \text{ S}_2\text{O}_3^{2-} + 4 \text{ H}^+ = \text{SeS}_4\text{O}_6^{2-} + \text{S}_4\text{O}_6^{2-} + 3 \text{ H}_2\text{O}$ (add small excess of thiosulfate and back-titrate with standard iodine solution) $\text{Na}_2\text{SeO}_3/4 = 47.23$                                                                                                                                                                                                           |
| $\text{SeO}_4^{2-}$ | $\text{SeO}_4^{2-} + 2 \text{ H}^+ + 2 \text{ Cl}^- = \text{SeO}_3^{2-} + \text{Cl}_2 + \text{H}_2\text{O}$ (absorb $\text{Cl}_2$ in KI solution)<br>$\text{Cl}_2 + 2 \text{ I}^- = 2 \text{ Cl}^- + \text{I}_2$ (titrate $\text{I}_2$ with standard thiosulfate) $\text{Na}_2\text{SeO}_4/2 = 94.47$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Sn(IV)              | $\text{SnCl}_6^{2-} + \text{Pb} = \text{Sn}^{2+} + \text{Pb}^{2+} + 6 \text{ Cl}^-$ (in $\text{CO}_2$ atmosphere boil 40 min)<br>$\text{Sn}^{2+} + \text{I}_2 + 6 \text{ Cl}^- = \text{SnCl}_6^{2-} + 2 \text{ I}^-$ (at $0\text{--}3^\circ\text{C}$ ) $\text{Sn}/2 = 59.35$ ; $\text{SnO}_2/2 = 67.35$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Sn(II)              | $\text{Sn(II)} + 2 \text{ Ce(IV)} = \text{Sn(IV)} + 2 \text{ Ce(III)}$ $\text{Sn}/2 = 59.35$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Te(IV)              | $3 \text{ H}_2\text{TeO}_3 + \text{Cr}_2\text{O}_7^{2-} + 8 \text{ H}^+ = 3 \text{ H}_2\text{TeO}_4 + 2 \text{ Cr}^{3+} + 4 \text{ H}_2\text{O}$ $\text{Te}/2 = 63.80$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Te(VI)              | $\text{H}_2\text{TeO}_4 + 2 \text{ Cl}^- + 2 \text{ H}^+ = \text{H}_2\text{TeO}_3 + \text{Cl}_2 + \text{H}_2\text{O}$ (see $\text{SeO}_4^{2-}$ ) $\text{Te}/2 = 63.80$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Ti                  | $2 \text{ Ti(IV)} + \text{Zn(reductor)} = 2 \text{ Ti(III)} + \text{Zn(II)}$<br>$\text{Ti(III)} + \text{Fe}^{3+} = \text{Ti(IV)} + \text{Fe}^{2+}$ (in $\text{CO}_2$ atmosphere; use KSCN as indicator) $\text{Ti}/1 = 47.88$<br>or<br>$\text{Ti(III)} + \text{Methylene blue} = \text{Ti(IV)} + \text{colorless leuco base}$ (in $\text{CO}_2$ atmosphere) $\text{Ti}/1 = 47.88$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| Tl                  | $2 \text{ Tl}^+ + \text{MnO}_4^- + 8 \text{ H}^+ = 2 \text{ Tl}^{3+} + \text{Mn}^{2+} + 4 \text{ H}_2\text{O}$ $\text{Tl}/2 = 102.19$<br>$\text{Tl}^+ + 2 \text{ Ce}^{3+} = \text{Tl}^{3+} + 2 \text{ Ce}^{3+}$ (to a yellow color or use 1,10-phenanthroline) $\text{Tl}/2 = 102.19$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| U                   | $\text{U(VI)} + \text{Zn} = \text{U(III)} + \text{U(IV)} + \text{Zn(II)}$ [pass air through solution to oxidize U(III) to U(IV)]<br>$5 \text{ U}^{4+} + 2 \text{ MnO}_4^- + 2 \text{ H}_2\text{O} = 5 \text{ UO}_2^{2+} + 2 \text{ Mn}^{2+} + 4 \text{ H}^+$ $\text{U}/2 = 119.01$ ; $\text{U}_3\text{O}_8/6 = 140.35$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| V                   | Oxidize V(IV) to V(V) with permanganate. Destroy excess with sodium azide and boiling.<br>$\text{VO}_2^+ + \text{Fe}^{2+} + 2 \text{ H}^+ = \text{VO}^{2+} + \text{Fe}^{3+} + \text{H}_2\text{O}$ (diphenylaminesulfonic acid indicator)<br>$\text{V}/1 = 50.94$<br>Reduce V(V) with $\text{SO}_2$ and bubble $\text{CO}_2$ through boiling solution to remove excess $\text{SO}_2$ .<br>$5 \text{ VO}^{2+} + \text{MnO}_4^- + \text{H}_2\text{O} = 5 \text{ VO}_2^+ + \text{Mn}^{2+} + 2 \text{ H}^+$ $\text{V}/1 = 50.94$<br>Reduce V(V) to V(II) with Zn; catch eluate in excess $\text{Fe}^{3+}$ .<br>$\text{V}^{2+} + 2 \text{ Fe}^{3+} + \text{H}_2\text{O} = \text{VO}^{2+} + 2 \text{ Fe}^{2+} + 2 \text{ H}^+$<br>Titrate $\text{VO}^{2+} \text{—Fe}^{2+}$ mixture with permanganate to $\text{VO}_2^+ \text{—Fe}^{3+}$ $\text{V}/3 = 16.98$ ; $\text{V}_2\text{O}_5/6 = 30.32$ |
| Zn                  | Dissolve precipitate of $\text{Zn}[\text{Hg}(\text{SCN})_4]$ in 4M HCl in stoppered flask, add $\text{CHCl}_3$ .<br>$2 \text{ SCN}^- + 3 \text{ IO}_3^- + 2 \text{ H}^+ + \text{CN}^- = 2 \text{ SO}_4^{2-} + 3 \text{ ICN} + \text{H}_2\text{O}$ $\text{Zn}/24 = 2.725$<br>$2 \text{ Fe}(\text{CN})_6^{3-} + 2 \text{ I}^- + 3 \text{ Zn}^{2+} + 2 \text{ K}^+ = \text{K}_2\text{Zn}_3[\text{Fe}(\text{CN})_6]_2 + \text{I}_2$<br>Remove $\text{I}_2$ as formed by standard thiosulfate solution.<br>$3 \text{ Zn}/2 = 98.07$ but empirical value of 99.07 is recommended.<br>Precipitate $\text{Zn}(\text{anthranilate})_2$ ; proceed as with Cd. $\text{Zn}/8 = 8.174$                                                                                                                                                                                                                |

**Note:** Additional procedural information plus interferences and general remarks will be found in J. A. Dean, ed., *Analytical Chemistry Handbook*, McGraw-Hill, New York, 1995.

### 11.6.5 Precipitation Titrations

Many precipitation reactions that are useful as separation techniques for gravimetric analysis fail to meet one or both of two requirements for titrimetry:

1. The reaction rate must be sufficiently rapid, particularly in the titration of dilute solutions and in the immediate vicinity of the end point. To increase the precipitation rate, it is sometimes beneficial to change solvents or to raise the temperature. By adding an excess of reagent and back-titrating, it may be possible to take advantage of a more rapid precipitation in the reverse direction. By choosing an end-point detection method that does not require equilibrium to be reached in the immediate vicinity of the end point, advantage may be taken of a faster reaction rate at points removed from the end point. Examples are: amperometric titrations, conductometric titrations, and photometric titrations.
2. The stoichiometry must be exact. Coprecipitation by solid-solution formation, foreign ion entrapment, and adsorption are possible sources of error.

Table 11.30 lists standard solutions for precipitation titrations and Table 11.31 lists specific reagents as indicators, adsorption indicators, and protective colloids for precipitation titrations.

### 11.6.6 Complexometric Titrations

A complexometric titration is based on the essentially stoichiometric reaction of a complexing agent (*chelon*) with another species to form a complex species (*chelonate*) that is only slightly dissociated and is soluble in the titration medium. In such a titration, either the chelon or the chelonate may serve as the limiting reagent (that is, as the titrant). The end point is detected by measuring or observing some property that reflects the change, in the vicinity of the equivalence point, in the concentration of the chelon or the chelonate. Examples of the application of metal-ion indicators are listed in Table 11.32. For a metal indicator to be useful, a proper sequence of effective stabilities must be met. On the one hand, the metal-indicator complex must be sufficiently stable to maintain itself in extremely dilute solution; otherwise the end-point color change will be spread over a broad interval of the titration, owing to the extended dissociation. On the other hand, the metal-indicator complex must be less stable than the metal chelonate; otherwise a sluggish end point, a late end point, or no end point at all will be obtained. Furthermore, the metal-indicator complex must react rapidly with the chelon. Only a limited number of the numerous chromogenic agents for metals allow this sequence and have useful indicator properties in chelometric titrations.

Among the complexing agents that find use as titrating agents, ethylenediamine-*N,N,N',N'*-tetraacetic acid (acronym EDTA, and equation abbreviation,  $H_4Y$ ) is by far the more important, and it is used in the vast majority of complexometric titrations. The successive acid  $pK_a$  values of  $H_4Y$  are  $pK_1 = 2.0$ ,  $pK_2 = 2.67$ ,  $pK_3 = 6.16$ ,  $pK_4 = 10.26$  at 20°C and an ionic strength of 0.1. The fraction  $\alpha_4$  present as the tetravalent anion is of particular importance in equilibrium calculations. Its magnitude at various pH values is given in Table 11.33.

The formation constants of EDTA complexes are gathered in Table 11.34. Based on their stability, the EDTA complexes of the most common metal ions may be roughly divided into three groups:

$\log K > 20$

Tri- and tetravalent cations including Bi, Fe(III), Ga, Hg(II), In, Sc, Th, U(IV), V(III), and Zr

$\log K = 15$  to 18

Divalent transition metals, rare earths, and Al

$\log K = 8$  to 11

Alkaline earths and Mg

The more stable the metal complex, the lower the pH at which it can be quantitatively formed. Elements in the first group may be titrated with EDTA at pH 1 to 3 without interference from cations of the last two groups, while cations of the second group may be titrated at pH 4 to 5 without interference from the alkaline earths.

In practice, an auxiliary complexing (masking) agent is usually added during EDTA titrations to prevent the precipitation of heavy metals as hydroxides or basic salts. The concentration of auxiliary complexing agents is generally high compared with the metal-ion concentration, and the solution is sufficiently well buffered so that the hydrogen ions produced during complexing of a metal ion by  $H_4Y$  do not cause an appreciable change in pH. Many EDTA titrations are carried out in ammonia–ammonium chloride buffers, which serve also to provide ammonia as an auxiliary complexing agent. The cumulative formation constants of ammine complexes are listed in Table 11.35.

**11.6.6.1 Types of Chelometric Titrations.** Chelometric titrations may be classified according to their manner of performance: direct titrations, back titrations, substitution titrations, redox titrations, or indirect methods.

**11.6.6.1.1 Direct Titrations.** The most convenient and simplest manner is the measured addition of a standard chelon solution to the sample solution (brought to the proper conditions of pH, buffer, etc.) until the metal ion is stoichiometrically chelated. Auxiliary complexing agents such as citrate, tartrate, or triethanolamine are added, if necessary, to prevent the precipitation of metal hydroxides or basic salts at the optimum pH for titration. For example, tartrate is added in the direct titration of lead. If a pH range of 9 to 10 is suitable, a buffer of ammonia and ammonium chloride is often added in relatively concentrated form, both to adjust the pH and to supply ammonia as an auxiliary complexing agent for those metal ions which form ammine complexes. A few metals, notably iron(III), bismuth, and thorium, are titrated in acid solution.

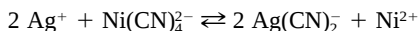
Direct titrations are commonly carried out using disodium dihydrogen ethylenediaminetetraacetate,  $Na_2H_2Y$ , which is available in pure form. The reaction of the chelon with the indicator must be rapid for a practical, direct titration. Where it is slow, heating of the titration medium is often expedient, or another indicator is employed.

**11.6.6.1.2 Back Titrations.** In the performance of a back titration, a known, but excess quantity of EDTA or other chelon is added, the pH is now properly adjusted, and the excess of the chelon is titrated with a suitable standard metal salt solution. Back titration procedures are especially useful when the metal ion to be determined cannot be kept in solution under the titration conditions or where the reaction of the metal ion with the chelon occurs too slowly to permit a direct titration, as in the titration of chromium(III) with EDTA. Back titration procedures sometimes permit a metal ion to be determined by the use of a metal indicator that is blocked by that ion in a direct titration. For example, nickel, cobalt, or aluminum form such stable complexes with Eriochrome Black T that the direct titration would fail. However, if an excess of EDTA is added before the indicator, no blocking occurs in the back titration with a magnesium or zinc salt solution. These metal ion titrants are chosen because they form EDTA complexes of relatively low stability, thereby avoiding the possible titration of EDTA bound by the sample metal ion.

In a back titration, a slight excess of the metal salt solution must sometimes be added to yield the color of the metal-indicator complex. Where metal ions are easily hydrolyzed, the complexing agent is best added at a suitable, low pH and only when the metal is fully complexed is the pH adjusted upward to the value required for the back titration. In back titrations, solutions of the following metal ions are commonly employed: Cu(II), Mg, Mn(II), Pb(II), Th(IV), and Zn. These solutions are usually prepared in the approximate strength desired from their nitrate salts (or the solution of the metal or its oxide or carbonate in nitric acid), and a minimum amount of acid is added to repress hydrolysis of the metal ion. The solutions are then standardized against an EDTA solution (or other chelon solution) of known strength.

**11.6.6.1.3 Substitution Titrations.** Upon the introduction of a substantial or equivalent amount of the chelonate of a metal that is less stable than that of the metal being determined, a substitution occurs, and the metal ion displaced can be titrated by the chelon in the same solution. This is a direct titration with regard to its performance, but in terms of the mechanism it can be considered as a substitution titration (or replacement titration).

In principle any ion can be used if it forms a weaker EDTA complex than the metal ion being determined. Still weaker metal-EDTA complexes would not interfere. Exchange reactions are also possible with other metal complexes to permit application of the chelometric titration to non-titrable cations and anions. The exchange reagent can be added and the titration performed in the sample solution without prior removal of the excess reagent. A most important example is the exchange of silver ion with an excess of the tetracyanonickelate ion according to the equation:

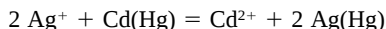


The nickel ion freed may then be determined by an EDTA titration. Note that two moles of silver are equivalent to one mole of nickel and thus to one mole of EDTA.

**11.6.6.1.4 Redox Titrations.** Redox titrations can be carried out in the presence of excess EDTA. Here EDTA acts to change the oxidation potential by forming a more stable complex with one oxidation state than with the other. Generally the oxidized form of the metal forms a more stable complex than the reduced form, and the couple becomes a stronger reducing agent in the presence of excess EDTA. For example, the Co(III)–Co(II) couple is shifted about 1.2 volts, so that Co(II) can be titrated with Ce(IV). Alternatively, Co(III) can be titrated to Co(II), with Cr(II) as a reducing agent.

Manganese(II) can be titrated directly to Mn(III) using hexacyanoferrate(III) as the oxidant. Alternatively, Mn(III), prepared by oxidation of the Mn(II)–EDTA complex with lead dioxide, can be determined by titration with standard iron(II) sulfate.

**11.6.6.1.5 Indirect Procedures.** Numerous inorganic anions that do not form complexes with a complexing agent are accessible to a chelometric titration by indirect procedures. Frequently the anion can be precipitated as a compound containing a stoichiometric amount of a titrable cation. Another indirect approach employing replacement mechanism is the reduction of a species with the liquid amalgam of a metal that can be determined by a chelometric titration after removal of excess amalgam. For example:



The equivalent amount of cadmium ion exchanged for the silver ion can readily be determined by EDTA titration procedures.

## 11.6.6.2 Preparation of Standard Solutions

**11.6.6.2.1 Standard EDTA Solutions.** Disodium dihydrogen ethylenediaminetetraacetate dihydrate is available commercially of analytical reagent purity. After drying at 80°C for at least 24 hr, its composition agrees exactly with the dihydrate formula (molecular weight 372.25). It may be weighed directly. If an additional check on the concentration is required, it may be standardized by titration with nearly neutralized zinc chloride or zinc sulfate solution.

**11.6.6.2.2 Standard Magnesium Solution.** Dissolve 24.647 g of magnesium sulfate heptahydrate in water and dilute to 1 L for 0.1M solution.

**11.6.6.2.3 Standard Manganese(II) Solution.** Dissolve exactly 16.901 g ACS reagent grade manganese(II) sulfate hydrate in water and dilute to 1 L.

**11.6.6.2.4 Standard Zinc Solution.** Dissolve exactly 13.629 g of zinc chloride, ACS reagent grade, or 28.754 g of zinc sulfate heptahydrate, and dilute to 1 L for 0.1000M solution.

**11.6.6.2.5 Buffer Solution, pH 10.** Add 142 mL of concentrated ammonia solution (sp. grav. 0.88–0.90) to 17.5 g of analytical reagent ammonium chloride, and dilute to 250 mL.

**11.6.6.2.6 Water.** Distilled water must be (a) redistilled in an all-Pyrex glass apparatus or (b) purified by passage through a column of cation exchange resin in the sodium form. For storage, polyethylene bottles are most satisfactory, particularly for very dilute (0.001M) EDTA solutions.

**11.6.6.2.7 Murexide Indicator.** Suspend 0.5 g of powdered murexide in water, shake thoroughly, and allow the undissolved solid to settle. Use 5–6 drops of the supernatant liquid for each titration. Decant the old supernatant liquid daily and treat the residue with water to provide a fresh solution of the indicator.

Alternatively, grind 0.1 g of murexide with 10 g of ACS reagent grade sodium chloride; use about 50 mg of the mixture for each titration.

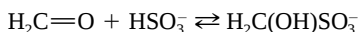
**11.6.6.2.8 Pyrocatechol Violet Indicator Solution.** Dissolve 0.1 g of the solid dyestuff in 100 mL of water.

## 11.6.7 Masking Agents

Masking (and demasking) techniques are widely used in analytical chemistry because they frequently provide convenient and elegant methods by which to avoid the effects of unwanted components of a system without having to resort to physical separation. The best molecules or ligands to use as masking agents are those that are chemically stable and nontoxic and react rapidly to form strong, colorless complexes with the ions to be masked, but form only relatively weak complexes with other ions that are present. Tables 11.36 and 11.37 are intended as qualitative guides to the types of masking agents likely to be suitable for particular analytical problems.

Masking must not be identified solely with complex formation. There are numerous complex compounds in which solutions show no masking effects. On the other hand, examples can be cited in which the product of soluble principal valence compounds may lead to masking. This latter category includes the annulment of the base action of  $\text{NH}_2$ — groups in carboxylic acids by the addition of formaldehyde, the masking of the iodometric oxidation of sulfites by formaldehyde, as well as the masking of almost all reactions of molybdenum(VI), tungsten(VI), and vanadium(V) by hydrogen peroxide or fluoride ion. Sometimes the masking agent changes the valence state of the metal ion. Examples include the reduction of Fe(III) to Fe(II) with hydrazine, hydroxylamine hydrochloride, or tin(II) chloride. Hydroxylamine also reduces Ce(IV) to Ce(III), Cu(II) to Cu(I), and Hg(II) to free Hg. Ascorbic acid reduces Cu(II) to Cu(I) in the presence of the chloride ion.

The reaction of the hydrogen sulfite ion in an alkaline solution with ketones and aldehydes is:



The carbon-oxygen double bond of the carbonyl group is opened, and the hydrogen sulfite radical is added. An increase in temperature reverses the reaction more easily for ketones than for aldehydes.

Certain organic substances have no charge at any pH but form complexes with substances that do have a charge. The sugars and polyalcohols form such complexes in the pH range between 9 and 10 with a number of anions; including borate, molybdate, and arsenite. Elegant ion exchange methods have been devised for the sugars.

Probably the most extensively applied masking agent is cyanide ion. In alkaline solution, cyanide forms strong cyano complexes with the following ions and masks their action toward EDTA: Ag, Cd, Co(II), Cu(II), Fe(II), Hg(II), Ni, Pd(II), Pt(II), Tl(III), and Zn. The alkaline earths, Mn(II), Pb, and the rare earths are virtually unaffected; hence, these latter ions may be titrated with EDTA with the former ions masked by cyanide. Iron(III) is also masked by cyanide. However, as the hexacyanoferrate(III) ion oxidizes many indicators, ascorbic acid is added to form hexacyanoferrate(II) ion. Moreover, since the addition of cyanide to an acidic solution results in the formation of deadly

hydrogen cyanide, the solution must first be made alkaline, with hydrous oxide formation prevented by the addition of tartrate. Zinc and cadmium may be demasked from their cyanide complexes by the action of formaldehyde.

Masking by oxidation or reduction of a metal ion to a state which does not react with EDTA is occasionally of value. For example, Fe(III) ( $\log K_{MY} = 24.23$ ) in acidic media may be reduced to Fe(II) ( $\log K_{MY} = 14.33$ ) by ascorbic acid; in this state iron does not interfere in the titration of some trivalent and tetravalent ions in strong acidic medium (pH 0 to 2). Similarly, Hg(II) can be reduced to the metal. In favorable conditions, Cr(III) may be oxidized by alkaline peroxide to chromate which does not complex with EDTA.

In resolving complex metal-ion mixtures, more than one masking or demasking process may be utilized with various aliquots of the sample solution, or applied simultaneously or stepwise with a single aliquot. In favorable cases, even four or five metals can be determined in a mixture by the application of direct and indirect masking processes. Of course, not all components of the mixture need be determined by chelometric titrations. For example, redox titrimetry may be applied to the determination of one or more of the metals present.

### 11.6.8 Demasking

For the major part, masking reactions that occur in solutions and lead to soluble compounds are equilibrium reactions. They usually require the use of an excess of the masking agent and can be reversed again by removal of the masking agent. The freeing of previously masked ionic or molecular species has been called *demasking*. This merits consideration in regard to its use in analysis. Masking never completely removes certain ionic or molecular species, but only reduces their concentrations. The extent of this lowering determines which color or precipitation reactions can be prevented. A system masked against a certain reagent is not necessarily masked against another but more aggressive reagent. It is therefore easy to see that masked reaction systems can also function as reagents at times (e.g., Fehling's solution, Nessler's reagent).

The methods used in demasking are varied. One approach is to change drastically the hydrogen ion concentration of the solution. The conditional stability constants of most metal complexes depend greatly on pH, so that simply raising or lowering the pH is frequently sufficient for selective demasking. In most cases a strong mineral acid is added, and the ligand is removed from the coordination sphere of the complex through the formation of a slightly ionized acid, as with the polyprotic (citric, tartaric, EDTA, and nitriloacetic) acids.

Another type of demasking involves formation of new complexes or other compounds that are more stable than the masked species. For example, boric acid is used to demask fluoride complexes of tin(IV) and molybdenum(VI). Formaldehyde is often used to remove the masking action of cyanide ions by converting the masking agent to a nonreacting species through the reaction:



which forms glycolic nitrile. Pertinent instances are the demasking of  $\text{Ni}(\text{CN})_4^{2-}$  ions to  $\text{Ni}^{2+}$  ions by formaldehyde and the demasking of dimethylglyoxime (dmg) from  $\text{Pd}(\text{dmg})_2^{2-}$  ions by cyanide. Selectivity is evident in that  $\text{Zn}(\text{CN})_4^{2-}$  is demasked whereas  $\text{Cu}(\text{CN})_3^-$  is not.

Destruction of the masking ligand by chemical reaction may be possible, as in the oxidation of EDTA in acid solutions by permanganate or another strong oxidizing agent. Hydrogen peroxide and Cu(II) ion destroy the tartrate complex of aluminum.

Demasking methods for a number of masking agents are enumerated in Table 11.38.



**TABLE 11.30** Standard Solutions for Precipitation Titrations

The list given below includes the substances that are most used and most useful for the standardization of solutions for precipitation titrations. Primary standard solutions are denoted by the letter (P) in Column 1.

| Standard                                                 | Formula weight | Preparation                                                                                                                                                                                                                                             |
|----------------------------------------------------------|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| AgNO <sub>3</sub> (P)                                    | 169.89         | Weigh the desired amount of ACS reagent grade* AgNO <sub>3</sub> , dried at 105°C for 2 hr, and dissolve in double distilled water. Store in amber container and away from light. Check against NaCl.                                                   |
| BaCl <sub>2</sub> · 2H <sub>2</sub> O                    | 244.28         | Dissolve clear crystals of the salt in distilled water. Standardize against K <sub>2</sub> SO <sub>4</sub> or Na <sub>2</sub> SO <sub>4</sub> .                                                                                                         |
| Hg(NO <sub>3</sub> ) <sub>2</sub> · H <sub>2</sub> O     | 342.62         | Dissolve the reagent grade salt in distilled water and dilute to desired volume. Standardize against NaCl.                                                                                                                                              |
| KBr                                                      | 119.01         | The commercial reagent (ACS) may contain 0.2% chloride. Prepare an aqueous solution of approximately the desired concentration and standardize it against AgNO <sub>3</sub> .                                                                           |
| K <sub>4</sub> [Fe(CN)] <sub>6</sub> · 3H <sub>2</sub> O | 422.41         | Dissolve the high-purity commercial salt in distilled water containing 0.2 g/L of Na <sub>2</sub> CO <sub>3</sub> . Kept in an amber container and away from direct sunlight, solutions are stable for a month or more. Standardize against zinc metal. |
| KSCN                                                     | 97.18          | Prepare aqueous solutions having the concentration desired. Standardize against AgNO <sub>3</sub> solution. Protect from direct sunlight.                                                                                                               |
| K <sub>2</sub> SO <sub>4</sub> (P)                       | 174.26         | Dissolve about 17.43 g, previously dried at 150°C and accurately weighed, in distilled water and dilute exactly to 1 L.                                                                                                                                 |
| NaCl (P)                                                 | 58.44          | Dry at 130–150°C and weigh accurately, from a closed container, 5.844 g, dissolve in water, and dilute exactly to 1 L.                                                                                                                                  |
| NaF (P)                                                  | 41.99          | Dry at 110°C and weigh the appropriate amount of ACS reagent. Dissolve in water and dilute exactly to 1 L.                                                                                                                                              |
| Na <sub>2</sub> SO <sub>4</sub> (P)                      | 142.04         | Weigh accurately 14.204 g, dried at 150°C, and dissolve in distilled water. Dilute to exactly 1 L.                                                                                                                                                      |
| Th(NO <sub>3</sub> ) <sub>4</sub> · 4H <sub>2</sub> O    | 552.12         | Weigh the appropriate amount of crystals and dissolve in water. Standardize against NaF.                                                                                                                                                                |

\* Meets standards of purity (and impurity) set by the American Chemical Society.

**TABLE 11.31** Indicators for Precipitation Titrations

| Indicator                                                        | Preparation and use                                                                                                                                                                                                              |
|------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Specific reagents                                                |                                                                                                                                                                                                                                  |
| $\text{NH}_4\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | Use reagent (ACS)* grade salt, low in chloride. Dissolve 175 g in 100 mL 6 M $\text{HNO}_3$ which has been gently boiled for 10 min to expel nitrogen oxides. Dilute with 500 mL water. Use 2 mL per 100 mL of end-point volume. |
| $\text{K}_2\text{CrO}_4$                                         | Use reagent (ACS)* grade salt, low in chloride. Prepare 0.1M aqueous solution (19.421 g/L). Use 2.5 mL per 100 mL of end-point volume.                                                                                           |
| Tetrahydroxy-1,4-benzoquinone (THQ)                              | Prepare fresh as required by dissolving 15 mg in 5 mL of water. Use 10 drops for each titration.                                                                                                                                 |
| Adsorption indicators                                            |                                                                                                                                                                                                                                  |
| Bromophenol blue                                                 | Dissolve 0.1 g of the acid in 200 mL 95% ethanol.                                                                                                                                                                                |
| 2',7'-Dichlorofluorescein                                        | Dissolve 0.1 g of the acid in 100 mL 70% ethanol. Use 1 mL for 100 mL of initial solution.                                                                                                                                       |
| Eosin, tetrabromofluorescein                                     | See Dichlorofluorescein.                                                                                                                                                                                                         |
| Fluorescein                                                      | Dissolve 0.4 g of the acid in 200 mL 70% ethanol. Use 10 drops.                                                                                                                                                                  |
| Potassium rhodizonate, $\text{C}_4\text{O}_4(\text{OK})_2$       | Prepare fresh as required by dissolving 15 mg in 5 mL of water. Use 10 drops for each titration.                                                                                                                                 |
| Rhodamine 6G                                                     | Dissolve 0.1 g in 200 mL 70% ethanol.                                                                                                                                                                                            |
| Sodium 3-alizarinsulfonate                                       | Prepare a 0.2% aqueous solution. Use 5 drops per 120 mL end-point volume.                                                                                                                                                        |
| Thorin                                                           | Prepare a 0.025% aqueous solution. Use 5 drops.                                                                                                                                                                                  |
| Protective colloids                                              |                                                                                                                                                                                                                                  |
| Dextrin                                                          | Use 5 mL of 2% aqueous solution of chloride-free dextrin per 25 mL of 0.1M halide solution.                                                                                                                                      |
| Polyethylene glycol 400                                          | Prepare a 50% (v/v) aqueous solution of the surfactant. Use 5 drops per 100 mL end-point volume.                                                                                                                                 |

\*Meets standards as set forth in *Reagent Chemicals*, American Chemical Society, Washington, D.C.; revised periodically.

**TABLE 11.32** Properties and Applications of Selected Metal Ion Indicators

| Indicator                                                                 | Chemical name                                                                                                                  | Dissociation constants and colors of free indicator species                                                                                                                                                                                   | Colors of metal-indicator complexes                                                                 | Applications                                                                                                                                                                                                                                  |
|---------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Calmagite<br>0.05 g/100 mL water; stable 1 year                           | 1-(6-Hydroxy- <i>m</i> -tolylazo)-2-naphthol-4-sulfonic acid                                                                   | H <sub>2</sub> In <sup>-</sup> (red); pK <sub>2</sub> = 8.1<br>HIn <sup>2-</sup> (blue); pK <sub>3</sub> = 12.4<br>In <sup>3-</sup> (orange)                                                                                                  | Wine-red                                                                                            | Titration performed with Eriochrome Black T as indicator may be carried out equally well with Calmagite                                                                                                                                       |
| Eriochrome Black T<br>0.1 g/100 mL water; prepare fresh daily             | 1-(2-Hydroxy-1-naphthyl-azo)-6-nitro-2-naphthol-4-sulfonic acid                                                                | H <sub>2</sub> In <sup>-</sup> (red); pK <sub>2</sub> = 6.3<br>HIn <sup>2-</sup> (blue); pK <sub>3</sub> = 11.5<br>In <sup>3-</sup> (yellow-orange)                                                                                           | Wine-red                                                                                            | <i>Direct titration:</i> Ba, Ca, Cd, In, Mg, Mn, Pb, Sc, Sr, Tl, Zn, and lanthanides<br><i>Back titration:</i> Al, Ba, Bi, Ca, Co, Cr, Fe, Ga, Hg, Mn, Ni, Pb, Pd, Sc, Tl, V<br><i>Substitution titration:</i> Au, Ba, Ca, Cu, Hg, Pb, Pd, Sr |
| Murexide<br>Suspend 0.5 g in water; use fresh supernatant liquid each day | 5-[(Hexahydro-2,4,6-trioxo-5-pyrimidinyl)imino]-2,4,6-(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i> )-pyrimidinetrione monoammonium salt | H <sub>4</sub> In <sup>-</sup> (red-violet); pK <sub>2</sub> = 9.2<br>H <sub>3</sub> In <sup>2-</sup> (violet); pK <sub>3</sub> = 10.9<br>H <sub>2</sub> In <sup>3-</sup> (blue)                                                              | Red with Ca <sup>2+</sup><br>Yellow with Co <sup>2+</sup> , Ni <sup>2+</sup> , and Cu <sup>2+</sup> | <i>Direct titration:</i> Ca, Co, Cu, Ni<br><i>Back titration:</i> Ca, Cr, Ga<br><i>Substitution titration:</i> Ag, Au, Pd                                                                                                                     |
| PAN                                                                       | 1-(2-Pyridylazo)-2-naphthol                                                                                                    | HIn (orange-red); pK <sub>1</sub> = 12.3<br>In <sup>-</sup> (pink)                                                                                                                                                                            | Red                                                                                                 | <i>Direct titration:</i> Cd, Cu, In, Sc, Tl, Zn<br><i>Back titration:</i> Cu, Fe, Ga, Ni, Pb, Sc, Sn, Zn<br><i>Substitution titration:</i> Al, Ca, Co, Fe, Ga, Hg, In, Mg, Mn, Ni, Pb, V, Zn                                                  |
| Pyrocatechol Violet<br>0.1 g/100 mL; stable several weeks                 | Pyrocatecholsulfonephthalein                                                                                                   | H <sub>4</sub> In (red); pK <sub>1</sub> = 0.2<br>H <sub>3</sub> In <sup>-</sup> (yellow); pK <sub>2</sub> = 7.8<br>H <sub>2</sub> In <sup>2-</sup> (violet); pK <sub>3</sub> = 9.8<br>HIn <sup>3-</sup> (red-purple); pK <sub>4</sub> = 11.7 | Blue, except red with Th(IV)                                                                        | <i>Direct titration:</i> Al, Bi, Cd, Co, Fe, Ga, Mg, Mn, Ni, Pb, Th, Zn<br><i>Back titration:</i> Al, Bi, Fe, Ga, In, Ni, Pd, Sn, Th, Ti                                                                                                      |
| Salicylic acid                                                            | 2-Hydroxybenzoic acid                                                                                                          | H <sub>2</sub> In; pK <sub>1</sub> = 2.98<br>HIn <sup>-</sup> ; pK <sub>2</sub> = 12.38                                                                                                                                                       | FeSCN <sup>2+</sup> at pH 3 is reddish-brown                                                        | Typical uses: Fe(III) titrated with EDTA to colorless iron-EDTA complex                                                                                                                                                                       |
| Xylenol orange                                                            | 3,3'-Bis[ <i>N,N</i> -di(carboxy-ethyl)aminomethyl]- <i>o</i> -cresolsulfonephthalein                                          | —COOH groups:<br>pK <sub>3</sub> = 0.76; pK <sub>4</sub> = 1.15;<br>pK <sub>5</sub> = 2.58; pK <sub>6</sub> = 3.23                                                                                                                            |                                                                                                     | Typical uses: Bi, Pb, Th                                                                                                                                                                                                                      |

**Source:** J. A. Dean, ed., *Analytical Chemistry Handbook*, McGraw-Hill, New York, 1995.

**TABLE 11.33** Variation of  $\alpha_4$  with pH

| pH  | $-\log \alpha_4$ | pH   | $-\log \alpha_4$ |
|-----|------------------|------|------------------|
| 2.0 | 13.44            | 7.0  | 3.33             |
| 2.5 | 11.86            | 8.0  | 2.29             |
| 3.0 | 10.60            | 9.0  | 1.29             |
| 4.0 | 8.48             | 10.0 | 0.46             |
| 5.0 | 6.45             | 11.0 | 0.07             |
| 6.0 | 4.66             | 12.0 | 0.00             |

**TABLE 11.34** Formation Constants of EDTA Complexes at 25°C, Ionic Strength Approaching Zero

| Metal ion | $\log K_{MY}$ | Metal ion | $\log K_{MY}$ |
|-----------|---------------|-----------|---------------|
| Co(III)   | 36            | V(IV)     | 18.0          |
| V(III)    | 25.9          | U(IV)     | 17.5          |
| In        | 24.95         | Ti(IV)    | 17.3          |
| Fe(III)   | 24.23         | Ce(III)   | 16.80         |
| Th        | 23.2          | Zn        | 16.4          |
| Sc        | 23.1          | Cd        | 16.4          |
| Cr(III)   | 23            | Co(II)    | 16.31         |
| Bi        | 22.8          | Al        | 16.13         |
| Tl(III)   | 22.5          | La        | 16.34         |
| Sn(II)    | 22.1          | Fe(II)    | 14.33         |
| Ti(III)   | 21.3          | Mn(II)    | 13.8          |
| Hg(II)    | 21.80         | Cr(II)    | 13.6          |
| Ga        | 20.25         | V(II)     | 12.7          |
| Zr        | 19.40         | Ca        | 11.0          |
| Cu(II)    | 18.7          | Be        | 9.3           |
| Ni        | 18.56         | Mg        | 8.64          |
| Pd(II)    | 18.5          | Sr        | 8.80          |
| Pb(II)    | 18.3          | Ba        | 7.78          |
| V(V)      | 18.05         | Ag        | 7.32          |

**TABLE 11.35** Cumulative Formation Constants of Ammine Complexes at 20°C, Ionic Strength 0.1

| Cation        | $\log K_1$ | $\log K_2$ | $\log K_3$ | $\log K_4$ | $\log K_5$ | $\log K_6$ |
|---------------|------------|------------|------------|------------|------------|------------|
| Cadmium       | 2.65       | 4.75       | 6.19       | 7.12       | 6.80       | 5.14       |
| Cobalt(II)    | 2.11       | 3.74       | 4.79       | 5.55       | 5.73       | 5.11       |
| Cobalt(III)   | 6.7        | 14.0       | 20.1       | 25.7       | 30.8       | 35.2       |
| Copper(I)     | 5.93       | 10.86      |            |            |            |            |
| Copper(II)    | 4.31       | 7.98       | 11.02      | 13.32      | 12.66      |            |
| Iron(II)      | 1.4        | 2.2        |            |            |            |            |
| Manganese(II) | 0.8        | 1.3        |            |            |            |            |
| Mercury(II)   | 8.8        | 17.5       | 18.5       | 19.28      |            |            |
| Nickel        | 2.80       | 5.04       | 6.77       | 7.96       | 8.71       | 8.74       |
| Platinum(II)  |            |            |            |            |            | 35.3       |
| Silver(I)     | 3.24       | 7.05       |            |            |            |            |
| Zinc          | 2.37       | 4.81       | 7.31       | 9.46       |            |            |

**TABLE 11.36** Masking Agents for Various Elements

| Element | Masking agent                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ag      | $\text{Br}^-$ , citrate, $\text{Cl}^-$ , $\text{CN}^-$ , $\text{I}^-$ , $\text{NH}_3$ , $\text{SCN}^-$ , $\text{S}_2\text{O}_3^{2-}$ , thiourea, thioglycolic acid, diethyldithiocarbamate, thiosemicarbazide, bis(2-hydroxyethyl)dithiocarbamate                                                                                                                                                                                                                                                                              |
| Al      | Acetate, acetylacetone, $\text{BF}_4^-$ , citrate, $\text{C}_2\text{O}_4^{2-}$ , EDTA, $\text{F}^-$ , formate, 8-hydroxyquinoline-5-sulfonic acid, mannitol, 2,3-mercaptopropanol, $\text{OH}^-$ , salicylate, sulfosalicylate, tartrate, triethanolamine, tiron                                                                                                                                                                                                                                                               |
| As      | Citrate, 2,3-dimercaptopropanol, $\text{NH}_2\text{OH} \cdot \text{HCl}$ , $\text{OH}^-$ , $\text{S}_2^{2-}$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate                                                                                                                                                                                                                                                                                                                                                                          |
| Au      | $\text{Br}^-$ , $\text{CN}^-$ , $\text{NH}_3$ , $\text{SCN}^-$ , $\text{S}_2\text{O}_3^{2-}$ , thiourea                                                                                                                                                                                                                                                                                                                                                                                                                        |
| Ba      | Citrate, cyclohexanediaminetetraacetic acid, <i>N,N</i> -dihydroxyethylglycine, EDTA, $\text{F}^-$ , $\text{SO}_4^{2-}$ , tartrate                                                                                                                                                                                                                                                                                                                                                                                             |
| Be      | Acetylacetone, citrate, EDTA, $\text{F}^-$ , sulfosalicylate, tartrate                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Bi      | $\text{Br}^-$ , citrate, $\text{Cl}^-$ , 2,3-dimercaptopropanol, dithizone, EDTA, $\text{I}^-$ , $\text{OH}^-$ , $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{SCN}^-$ , tartrate, thiosulfate, thiourea, triethanolamine                                                                                                                                                                                                                                                                                                      |
| Ca      | $\text{BF}_4^-$ , citrate, <i>N,N</i> -dihydroxyethylglycine, EDTA, $\text{F}^-$ , polyphosphates, tartrate                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Cd      | Citrate, $\text{CN}^-$ , 2,3-dimercaptopropanol, dimercaptosuccinic acid, dithizone, EDTA, glycine, $\text{I}^-$ , malonate, $\text{NH}_3$ , 1,10-phenanthroline, $\text{SCN}^-$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate                                                                                                                                                                                                                                                                                                      |
| Ce      | Citrate, <i>N,N</i> -dihydroxyethylglycine, EDTA, $\text{F}^-$ , $\text{PO}_4^{3-}$ , reducing agents (ascorbic acid), tartrate, tiron                                                                                                                                                                                                                                                                                                                                                                                         |
| Co      | Citrate, $\text{CN}^-$ , diethyldithiocarbamate, 2,3-dimercaptopropanol, dimethylglyoxime, ethylenediamine, EDTA, $\text{F}^-$ , glycine, $\text{H}_2\text{O}_2$ , $\text{NH}_3$ , $\text{NO}_2^-$ , 1,10-phenanthroline, $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{SCN}^-$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate                                                                                                                                                                                                       |
| Cr      | Acetate, (reduction with) ascorbic acid + KI, citrate, <i>N,N</i> -dihydroxyethylglycine, EDTA, $\text{F}^-$ , formate, $\text{NaOH} + \text{H}_2\text{O}_2$ , oxidation to $\text{CrO}_4^{2-}$ , $\text{Na}_5\text{P}_3\text{O}_{10}$ , sulfosalicylate, tartrate, triethylamine, tiron                                                                                                                                                                                                                                       |
| Cu      | Ascorbic acid + KI, citrate, $\text{CN}^-$ , diethyldithiocarbamate, 2,3-dimercaptopropanol, ethylenediamine, EDTA, glycine, hexacyanocobalt(III)(3-), hydrazine, $\text{I}^-$ , $\text{NaH}_2\text{PO}_2$ , $\text{NH}_2\text{OH} \cdot \text{HCl}$ , $\text{NH}_3$ , $\text{NO}_2^-$ , 1,10-phenanthroline, $\text{S}^{2-}$ , $\text{SCN}^- + \text{SO}_3^{2-}$ , $\text{S}_2\text{O}_3^{2-}$ , sulfosalicylate, tartrate, thioglycolic acid, thiosemicarbazide, thiocarbohydrazide, thiourea                                |
| Fe      | Acetylacetone, (reduction with) ascorbic acid, $\text{C}_2\text{O}_4^{2-}$ , citrate, $\text{CN}^-$ , 2,3-dimercaptopropanol, EDTA, $\text{F}^-$ , $\text{NH}_3$ , $\text{NH}_2\text{OH} \cdot \text{HCl}$ , $\text{OH}^-$ , oxine, 1,10-phenanthroline, 2,2'-bipyridyl, $\text{PO}_4^{3-}$ , $\text{P}_2\text{O}_7^{4-}$ , $\text{S}^{2-}$ , $\text{SCN}^-$ , $\text{SnCl}_2$ , $\text{S}_2\text{O}_3^{2-}$ , sulfamic acid, sulfosalicylate, tartrate, thioglycolic acid, thiourea, tiron, triethanolamine, trithiocarbonate |
| Ga      | Citrate, $\text{Cl}^-$ , EDTA, $\text{OH}^-$ , oxalate, sulfosalicylate, tartrate                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| Ge      | $\text{F}^-$ , oxalate, tartrate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Hf      | See Zr                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Hg      | Acetone, (reduction with) ascorbic acid, citrate, $\text{Cl}^-$ , $\text{CN}^-$ , 2,3-dimercaptopropan-1-ol, EDTA, formate, $\text{I}^-$ , $\text{SCN}^-$ , $\text{SO}_3^{2-}$ , tartrate, thiosemicarbazide, thiourea, triethanolamine                                                                                                                                                                                                                                                                                        |
| In      | $\text{Cl}^-$ , EDTA, $\text{F}^-$ , $\text{SCN}^-$ , tartrate, thiourea, triethanolamine                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Ir      | Citrate, $\text{CN}^-$ , $\text{SCN}^-$ , tartrate, thiourea                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| La      | Citrate, EDTA, $\text{F}^-$ , oxalate, tartrate, tiron                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Mg      | Citrate, $\text{C}_2\text{O}_4^{2-}$ , cyclohexane-1,2-diaminetetraacetic acid, <i>N,N</i> -dihydroxyethylglycine, EDTA, $\text{F}^-$ , glycol, hexametaphosphate, $\text{OH}^-$ , $\text{P}_2\text{O}_7^{4-}$ , triethanolamine                                                                                                                                                                                                                                                                                               |
| Mn      | Citrate, $\text{CN}^-$ , $\text{C}_2\text{O}_4^{2-}$ , 2,3-dimercaptopropanol, EDTA, $\text{F}^-$ , $\text{Na}_5\text{P}_3\text{O}_{10}$ , oxidation to $\text{MnO}_4^-$ , $\text{P}_2\text{O}_7^{4-}$ , reduction to Mn(II) with $\text{NH}_2\text{OH} \cdot \text{HCl}$ or hydrazine, sulfosalicylate, tartrate, triethanolamine, triphosphate, tiron                                                                                                                                                                        |
| Mo      | Acetylacetone, ascorbic acid, citrate, $\text{C}_2\text{O}_4^{2-}$ , EDTA, $\text{F}^-$ , $\text{H}_2\text{O}_2$ , hydrazine, mannitol, $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{NH}_2\text{OH} \cdot \text{HCl}$ , oxidation to molybdate, $\text{SCN}^-$ , tartrate, tiron, triphosphate                                                                                                                                                                                                                                |

**TABLE 11.36** Masking Agents for Various Elements (*Continued*)

| Element         | Masking agent                                                                                                                                                                                                                                                                                                                                      |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Nb              | Citrate, $\text{C}_2\text{O}_4^{2-}$ , $\text{F}^-$ , $\text{H}_2\text{O}_2$ , $\text{OH}^-$ , tartrate                                                                                                                                                                                                                                            |
| Nd              | EDTA                                                                                                                                                                                                                                                                                                                                               |
| $\text{NH}_4^+$ | HCHO                                                                                                                                                                                                                                                                                                                                               |
| Ni              | Citrate, $\text{CN}^-$ , <i>N,N</i> -dihydroxyethylglycine, dimethylglyoxime, EDTA, $\text{F}^-$ , glycine, malonate, $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{NH}_3$ , 1,10-phenanthroline, $\text{SCN}^-$ , sulfosalicylate, thioglycolic acid, triethanolamine, tartrate                                                                   |
| Np              | $\text{F}^-$                                                                                                                                                                                                                                                                                                                                       |
| Os              | $\text{CN}^-$ , $\text{SCN}^-$ , thiourea                                                                                                                                                                                                                                                                                                          |
| Pa              | $\text{H}_2\text{O}_2$                                                                                                                                                                                                                                                                                                                             |
| Pb              | Acetate, $(\text{C}_6\text{H}_5)_4\text{AsCl}$ , citrate, 2,3-dimercaptopropanol, EDTA, $\text{I}^-$ , $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{SO}_4^{2-}$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate, tiron, tetraphenylarsonium chloride, triethanolamine, thioglycolic acid                                                                 |
| Pd              | Acetylacetone, citrate, $\text{CN}^-$ , EDTA, $\text{I}^-$ , $\text{NH}_3$ , $\text{NO}_2^-$ , $\text{SCN}^-$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate, triethanolamine                                                                                                                                                                            |
| Pt              | Citrate, $\text{CN}^-$ , EDTA, $\text{I}^-$ , $\text{NH}_3$ , $\text{NO}_2^-$ , $\text{SCN}^-$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate, urea                                                                                                                                                                                                      |
| Pu              | Reduction to Pu(IV) with sulfamic acid                                                                                                                                                                                                                                                                                                             |
| Rare earths     | $\text{C}_2\text{O}_4^{2-}$ , citrate, EDTA, $\text{F}^-$ , tartrate                                                                                                                                                                                                                                                                               |
| Re              | Oxidation to perrhenate                                                                                                                                                                                                                                                                                                                            |
| Rh              | Citrate, tartrate, thiourea                                                                                                                                                                                                                                                                                                                        |
| Ru              | $\text{CN}^-$ , thiourea                                                                                                                                                                                                                                                                                                                           |
| Sb              | Citrate, 2,3-dimercaptopropanol, EDTA, $\text{F}^-$ , $\text{I}^-$ , $\text{OH}^-$ , oxalate, $\text{S}^{2-}$ , $\text{S}_2^{2-}$ , $\text{S}_2\text{O}_3^{2-}$ , tartrate, triethanolamine                                                                                                                                                        |
| Sc              | Cyclohexane-1,2-diaminetetraacetic acid, $\text{F}^-$ , tartrate                                                                                                                                                                                                                                                                                   |
| Se              | Citrate, $\text{F}^-$ , $\text{I}^-$ , reducing agents, $\text{S}^{2-}$ , $\text{SO}_3^{2-}$ , tartrate                                                                                                                                                                                                                                            |
| Sn              | Citrate, $\text{C}_2\text{O}_3^{3-}$ , 2,3-dimercaptopropanol, EDTA, $\text{F}^-$ , $\text{I}^-$ , $\text{OH}^-$ , oxidation with bromine water, phosphate(3-), tartrate, triethanolamine, thioglycolic acid                                                                                                                                       |
| Sr              | Citrate, <i>N,N</i> -dihydroxyethylglycine, EDTA, $\text{F}^-$ , $\text{SO}_4^{2-}$ , tartrate                                                                                                                                                                                                                                                     |
| Ta              | Citrate, $\text{F}^-$ , $\text{H}_2\text{O}_2$ , $\text{OH}^-$ , oxalate, tartrate                                                                                                                                                                                                                                                                 |
| Te              | Citrate, $\text{F}^-$ , $\text{I}^-$ , reducing agents, $\text{S}^{2-}$ , sulfite, tartrate                                                                                                                                                                                                                                                        |
| Th              | Acetate, acetylacetone, citrate, EDTA, $\text{F}^-$ , $\text{SO}_4^{2-}$ , 4-sulfobenzeneearsonic acid, sulfosalicylic acid, tartrate, triethanolamine                                                                                                                                                                                             |
| Ti              | Ascorbic acid, citrate, $\text{F}^-$ , gluconate, $\text{H}_2\text{O}_2$ , mannitol, $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{OH}^-$ , $\text{SO}_4^{2-}$ , sulfosalicylic acid, tartrate, triethanolamine, tiron                                                                                                                             |
| Tl              | Citrate, $\text{Cl}^-$ , $\text{CN}^-$ , EDTA, HCHO, hydrazine, $\text{NH}_2\text{OH} \cdot \text{HCl}$ , oxalate, tartrate, triethanolamine                                                                                                                                                                                                       |
| U               | Citrate, $(\text{NH}_4)_2\text{CO}_3$ , $\text{C}_2\text{O}_4^{2-}$ , EDTA, $\text{F}^-$ , $\text{H}_2\text{O}_2$ , hydrazine + triethanolamine, phosphate(3-), tartrate                                                                                                                                                                           |
| V               | (Reduction with) ascorbic acid, hydrazine, or $\text{NH}_2\text{OH} \cdot \text{HCl}$ , $\text{CN}^-$ , EDTA, $\text{F}^-$ , $\text{H}_2\text{O}_2$ , mannitol, oxidation to vanadate, triethanolamine, tiron                                                                                                                                      |
| W               | Citrate, $\text{F}^-$ , $\text{H}_2\text{O}_2$ , hydrazine, $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{NH}_2\text{OH} \cdot \text{HCl}$ , oxalate, $\text{SCN}^-$ , tartrate, tiron, triphosphate, oxidation to tungstate(VI)                                                                                                                   |
| Y               | Cyclohexane-1,2-diaminetetraacetic acid, $\text{F}^-$                                                                                                                                                                                                                                                                                              |
| Zn              | Citrate, $\text{CN}^-$ , <i>N,N</i> -dihydroxyethylglycine, 2,3-dimercaptopropanol, dithizone, EDTA, $\text{F}^-$ , glycerol, glycol, hexacyanoferrate(II)(4-), $\text{Na}_5\text{P}_3\text{O}_{10}$ , $\text{NH}_3$ , $\text{OH}^-$ , $\text{SCN}^-$ , tartrate, triethanolamine                                                                  |
| Zr              | Arsenazo, carbonate, citrate, $\text{C}_2\text{O}_4^{2-}$ , cyclohexane-1,2-diaminetetraacetic acid, EDTA, $\text{F}^-$ , $\text{H}_2\text{O}_2$ , $\text{PO}_4^{3-}$ , $\text{P}_2\text{O}_5^{2-}$ , pyrogallol, quinalizarinesulfonic acid, salicylate, $\text{SO}_4^{2-}$ + $\text{H}_2\text{O}_2$ , sulfosalicylate, tartrate, triethanolamine |

TABLE 11.37 Masking Agents for Anions and Neutral Molecules

| Anion or neutral molecule         | Masking agent                                                                                                      |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------|
| Boric acid                        | F <sup>-</sup> , glycol, mannitol, tartrate, and other hydroxy acids                                               |
| Br <sup>-</sup>                   | Hg(II)                                                                                                             |
| Br <sub>2</sub>                   | Phenol, sulfosalicylic acid                                                                                        |
| BrO <sub>3</sub> <sup>-</sup>     | Reduction with arsenate(III), hydrazine, sulfite, or thiosulfate                                                   |
| Chromate(VI)                      | Reduction with arsenate(III), ascorbic acid, hydrazine, hydroxylamine, sulfite, or thiosulfate                     |
| Citrate                           | Ca(II)                                                                                                             |
| Cl <sup>-</sup>                   | Hg(II), Sb(III)                                                                                                    |
| Cl <sub>2</sub>                   | Sulfite                                                                                                            |
| ClO <sub>3</sub> <sup>-</sup>     | Thiosulfate                                                                                                        |
| ClO <sub>4</sub> <sup>-</sup>     | Hydrazine, sulfite                                                                                                 |
| CN <sup>-</sup>                   | HCHO, Hg(II), transition metal ions                                                                                |
| EDTA                              | Cu(II)                                                                                                             |
| F <sup>-</sup>                    | Al(III), Be(II), boric acid, Fe(III), Th(IV), Ti(IV), Zr(IV)                                                       |
| Fe(CN) <sub>6</sub> <sup>3-</sup> | Arsenate(III), ascorbic acid, hydrazine, hydroxylamine, thiosulfate                                                |
| Germanic acid                     | Glucose, glycerol, mannitol                                                                                        |
| I <sup>-</sup>                    | Hg(II)                                                                                                             |
| I <sub>2</sub>                    | Thiosulfate                                                                                                        |
| IO <sub>3</sub> <sup>-</sup>      | Hydrazine, sulfite, thiosulfate                                                                                    |
| IO <sub>4</sub> <sup>-</sup>      | Arsenate(III), hydrazine, molybdate(VI), sulfite, thiosulfate                                                      |
| MnO <sub>4</sub> <sup>-</sup>     | Reduction with arsenate(III), ascorbic acid, azide, hydrazine, hydroxylamine, oxalic acid, sulfite, or thiosulfate |
| MoO <sub>4</sub> <sup>2-</sup>    | Citrate, F <sup>-</sup> , H <sub>2</sub> O <sub>2</sub> , oxalate, thiocyanate + Sn(II)                            |
| NO <sub>2</sub> <sup>-</sup>      | Co(II), sulfamic acid, sulfanilic acid, urea                                                                       |
| Oxalate                           | Molybdate(VI), permanganate                                                                                        |
| Phosphate                         | Fe(III), tartrate                                                                                                  |
| S                                 | CN <sup>-</sup> , S <sup>2-</sup> , sulfite                                                                        |
| S <sup>2-</sup>                   | Permanganate + sulfuric acid, sulfur                                                                               |
| Sulfate                           | Cr(III) + heat                                                                                                     |
| Sulfite                           | HCHO, Hg(II), permanganate + sulfuric acid                                                                         |
| SO <sub>5</sub> <sup>2-</sup>     | Ascorbic acid, hydroxylamine, thiosulfate                                                                          |
| Se and its anions                 | Diaminobenzidine, sulfide, sulfite                                                                                 |
| Te                                | I <sup>-</sup>                                                                                                     |
| Tungstate                         | Citrate, tartrate                                                                                                  |
| Vanadate                          | Tartrate                                                                                                           |

TABLE 11.38 Common Demasking Agents

Abbreviations: DPC, diphenylcarbazide; HDMG, dimethylglyoxime; PAN, 1-(2-pyridylazo)-2-naphthol.

| Complexing agent | Ion demasked     | Demasking agent        | Application                                  |
|------------------|------------------|------------------------|----------------------------------------------|
| CN <sup>-</sup>  | Ag <sup>+</sup>  | H <sup>+</sup>         | Precipitation of Ag                          |
|                  | Cd <sup>2+</sup> | H <sup>+</sup>         | Free Cd <sup>2+</sup>                        |
|                  |                  | HCHO + OH <sup>-</sup> | Detection of Cd (with DPC) in presence of Cu |
|                  |                  | H <sup>+</sup>         | Precipitation of Cu                          |
|                  | Cu <sup>2+</sup> | HgO                    | Determination of Cu                          |
|                  | Fe <sup>2+</sup> | Hg <sup>2+</sup>       | Free Fe <sup>2+</sup>                        |
|                  | Fe <sup>3+</sup> | HgO                    | Determination of Fe                          |
|                  |                  |                        |                                              |

**TABLE 11.38** Common Demasking Agents (*Continued*)

| Complexing agent                                                                                     | Ion demasked          | Demasking agent                                     | Application                                                                             |
|------------------------------------------------------------------------------------------------------|-----------------------|-----------------------------------------------------|-----------------------------------------------------------------------------------------|
| $\text{CN}^-$ ( <i>continued</i> )                                                                   | HDMG                  | $\text{Pd}^{2+}$                                    | Detection of $\text{CN}^-$ (with $\text{Ni}^{2+}$ )                                     |
|                                                                                                      | $\text{Hg}^{2+}$      | $\text{Pd}^{2+}$                                    | Detection of Pd (with DPC)                                                              |
|                                                                                                      | $\text{Ni}^{2+}$      | HCHO                                                | Detection of Ni (with HDMG)                                                             |
|                                                                                                      |                       | $\text{H}^+$                                        | Free $\text{Ni}^{2+}$                                                                   |
|                                                                                                      |                       | HgO                                                 | Determination of Ni                                                                     |
|                                                                                                      |                       | $\text{Ag}^+$                                       | Detection and determination of Ni (with HDMG) in presence of Co                         |
|                                                                                                      |                       | $\text{Ag}^+$ , $\text{Hg}^{2+}$ , $\text{Pb}^{2+}$ | Detection of Ag, Hg, Pb (with HDMG)                                                     |
|                                                                                                      | $\text{Pd}^{2+}$      | $\text{H}^+$                                        | Precipitation of Pd                                                                     |
|                                                                                                      |                       | HgO                                                 | Determination of Pd                                                                     |
|                                                                                                      | $\text{Zn}^{2+}$      | $\text{Cl}_3\text{CCHO} \cdot \text{H}_2\text{O}$   | Titration of Zn with EDTA                                                               |
| $\text{CO}_3^{2-}$<br>$\text{C}_2\text{O}_4^{2-}$<br>$\text{Cl}^-$ (concentrated)<br>Ethylenediamine |                       | $\text{H}^+$                                        | Free Zn                                                                                 |
|                                                                                                      | $\text{Cu}^{2+}$      | $\text{H}^+$                                        | Free $\text{Cu}^{2+}$                                                                   |
|                                                                                                      | $\text{Al}^{3+}$      | $\text{OH}^-$                                       | Precipitation of $\text{Al}(\text{OH})_3$                                               |
|                                                                                                      | $\text{Ag}^+$         | $\text{H}_2\text{O}$                                | Precipitation of AgCl                                                                   |
|                                                                                                      | $\text{Ag}^+$         | $\text{SiO}_2$ (amorphous)                          | Differentiation of crystalline and amorphous $\text{SiO}_2$ (with $\text{CrO}_4^{2-}$ ) |
|                                                                                                      |                       |                                                     | Titration of Al                                                                         |
| EDTA                                                                                                 | $\text{Al}^{3+}$      | $\text{F}^-$                                        | Precipitation of $\text{BaSO}_4$ (with $\text{SO}_4^{2-}$ )                             |
|                                                                                                      | $\text{Ba}^{2+}$      | $\text{H}^+$                                        | Detection of Co (with diethyldithiocarbamate)                                           |
|                                                                                                      | $\text{Co}^{2+}$      | $\text{Ca}^{2+}$                                    | Titration of Mg, Mn                                                                     |
|                                                                                                      | $\text{Mg}^{2+}$      | $\text{F}^-$                                        | Titration of Th                                                                         |
|                                                                                                      | Th(IV)                | $\text{SO}_4^{2-}$                                  | Precipitation of Ti (with $\text{NH}_3$ )                                               |
|                                                                                                      | Ti(IV)                | $\text{Mg}^{2+}$                                    | Titration of Mg, Mn, Zn                                                                 |
|                                                                                                      | $\text{Zn}^{2+}$      | $\text{CN}^-$                                       | Free ions                                                                               |
|                                                                                                      | Many ions             | $\text{KMO}_4^-$                                    | Precipitation of Al (with 8-hydroxyquinoline)                                           |
|                                                                                                      | Al(III)               | Be(II)                                              | Precipitation of $\text{Al}(\text{OH})_3$                                               |
|                                                                                                      |                       | $\text{OH}^-$                                       | Precipitation of $\text{Fe}(\text{OH})_3$                                               |
| $\text{F}^-$                                                                                         | Fe(III)               | $\text{OH}^-$                                       | Detection of Hg (with xylenol orange)                                                   |
|                                                                                                      | Hf(IV)                | Al(III) or Be(II)                                   | Free molybdate                                                                          |
|                                                                                                      | Mo(VI)                | $\text{H}_3\text{BO}_3$                             | Precipitation of Sn (with $\text{H}_2\text{S}$ )                                        |
|                                                                                                      | Sn(IV)                | $\text{H}_3\text{BO}_3$                             | Detection of U (with dibenzoylmethane)                                                  |
|                                                                                                      | U(VI)                 | Al(III)                                             | Detection of Zr (with xylenol orange)                                                   |
|                                                                                                      |                       | Ca(II)                                              | Detection of Ca (with alizarin S)                                                       |
|                                                                                                      |                       | $\text{OH}^-$                                       | Precipitation of $\text{Zr}(\text{OH})_4$                                               |
|                                                                                                      | Zr(IV)                | Al(III) or Be(II)                                   | Free ions                                                                               |
|                                                                                                      |                       | Fe(III)                                             |                                                                                         |
|                                                                                                      |                       |                                                     |                                                                                         |
| $\text{H}_2\text{O}_2$                                                                               | Hf(IV), Ti(IV), or Zr |                                                     |                                                                                         |
| $\text{NH}_3$                                                                                        | $\text{Ag}^+$         | $\text{Br}^-$                                       | Detection of $\text{Br}^-$                                                              |
|                                                                                                      |                       | $\text{H}^+$                                        | Detection of Ag                                                                         |
|                                                                                                      |                       | $\text{I}^-$                                        | Detection of I and Br                                                                   |
|                                                                                                      |                       | $\text{SiO}_2$ (amorphous)                          | Differentiation of crystalline and amorphous $\text{SiO}_2$ (with $\text{CrO}_4^{2-}$ ) |
|                                                                                                      |                       |                                                     | Free Co                                                                                 |
| $\text{NO}_2^-$                                                                                      | Co(III)               | $\text{H}^+$                                        | Precipitation of $\text{FePO}_4$                                                        |
| $\text{PO}_4^{3-}$                                                                                   | Fe(III)               | $\text{OH}^-$                                       | Detection of U (with dibenzoylmethane)                                                  |
|                                                                                                      | $\text{UO}_2^{2+}$    | Al(III)                                             | Precipitation of $\text{Fe}(\text{OH})_3$                                               |
|                                                                                                      |                       |                                                     | Precipitation of $\text{BaSO}_4$                                                        |
| $\text{SCN}^-$                                                                                       | Fe(III)               | $\text{OH}^-$                                       | Free $\text{Ag}^+$                                                                      |
| $\text{SO}_4^{2-}$ (conc. $\text{H}_2\text{SO}_4$ )                                                  | $\text{Ba}^{2+}$      | $\text{H}_2\text{O}$                                | Detection of Cu (with PAN)                                                              |
| $\text{S}_2\text{O}_3^{2-}$                                                                          | $\text{Ag}^+$         | $\text{H}^+$                                        | Precipitation of Al(III)                                                                |
|                                                                                                      | $\text{Cu}^{2+}$      | $\text{OH}^-$                                       |                                                                                         |
| Tartrate                                                                                             | Al(III)               | $\text{H}_2\text{O}_2 + \text{Cu}^{2+}$             |                                                                                         |



**TABLE 11.39** Amino Acids pI and pK<sub>a</sub> Values

This table lists the pK<sub>a</sub> and pI (pH at the isoelectric point) values of α-amino acids commonly found in proteins along with their abbreviations. The dissociation constants refer to aqueous solutions at 25°C.

| Name          | Abbreviations |          | pK <sub>a</sub> values |                               |              | pI values |
|---------------|---------------|----------|------------------------|-------------------------------|--------------|-----------|
|               | 3 Letter      | 1 Letter | —COOH                  | —NH <sub>3</sub> <sup>+</sup> | Other groups |           |
| Alanine       | Ala           | A        | 2.34                   | 9.69                          |              | 6.00      |
| Arginine      | Arg           | R        | 2.17                   | 9.04                          | 12.48        | 10.76     |
| Asparagine    | Asn           | N        | 2.01                   | 8.80                          |              | 5.41      |
| Aspartic acid | Asp           | D        | 1.89                   | 9.60                          | 3.65         | 2.77      |
| Cysteine      | Cys           | C        | 1.96                   | 10.28                         | 8.18         | 5.07      |
| Glutamine     | Gln           | Q        | 2.17                   | 9.13                          |              | 5.65      |
| Glutamic acid | Glu           | E        | 2.19                   | 9.67                          | 4.25         | 3.22      |
| Glycine       | Gly           | G        | 2.34                   | 9.60                          |              | 5.97      |
| Histidine     | His           | H        | 1.82                   | 9.17                          | 6.00         | 7.59      |
| Isoleucine    | Ile           | I        | 2.36                   | 9.60                          |              | 6.02      |
| Leucine       | Leu           | L        | 2.36                   | 9.60                          | 5.98         |           |
| Lysine        | Lys           | K        | 2.18                   | 8.98                          | 10.53        | 9.74      |
| Methionine    | Met           | M        | 2.28                   | 9.21                          |              | 5.74      |
| Phenylalanine | Phe           | F        | 1.83                   | 9.13                          |              | 5.48      |
| Proline       | Pro           | P        | 1.99                   | 10.60                         |              | 6.30      |
| Serine        | Ser           | S        | 2.21                   | 9.15                          |              | 5.68      |
| Threonine     | Thr           | T        | 2.09                   | 9.10                          |              | 5.60      |
| Tryptophan    | Trp           | W        | 2.83                   | 9.39                          |              | 5.89      |
| Tyrosine      | Tyr           | Y        | 2.20                   | 9.11                          | 10.07        | 5.66      |
| Valine        | Val           | V        | 2.32                   | 9.62                          |              | 5.96      |

**Source:** E. L. Smith, et al., *Principles of Biochemistry*, 7th ed., McGraw-Hill, New York, 1983; H. J. Hinz, ed., *Thermodynamic Data for Biochemistry and Biotechnology*, Springer-Verlag, Heidelberg, 1986.

**TABLE 11.40** Tolerances of Volumetric Flasks

| Capacity, mL | Tolerances,* ±mL |         | Capacity, mL | Tolerances,* ±mL |         |
|--------------|------------------|---------|--------------|------------------|---------|
|              | Class A          | Class B |              | Class A          | Class B |
| 5            | 0.02             | 0.04    | 200          | 0.10             | 0.20    |
| 10           | 0.02             | 0.04    | 250          | 0.12             | 0.24    |
| 25           | 0.03             | 0.06    | 500          | 0.20             | 0.40    |
| 50           | 0.05             | 0.10    | 1000         | 0.30             | 0.60    |
| 100          | 0.08             | 0.16    | 2000         | 0.50             | 1.00    |

\*Accuracy tolerances for volumetric flasks at 20°C are given by ASTM standard E288.

**TABLE 11.41** Pipet Capacity Tolerances

| Volumetric transfer pipets |                       |         | Measuring and serological pipets |                       |
|----------------------------|-----------------------|---------|----------------------------------|-----------------------|
| Capacity, mL               | Tolerances,* $\pm$ mL |         | Capacity, mL                     | Tolerances,† $\pm$ mL |
|                            | Class A               | Class B |                                  | Class B               |
| 0.5                        | 0.006                 | 0.012   | 0.1                              | 0.005                 |
| 1                          | 0.006                 | 0.012   | 0.2                              | 0.008                 |
| 2                          | 0.006                 | 0.012   | 0.25                             | 0.008                 |
| 3                          | 0.01                  | 0.02    | 0.5                              | 0.01                  |
| 4                          | 0.01                  | 0.02    | 0.6                              | 0.01                  |
| 5                          | 0.01                  | 0.02    | 1                                | 0.02                  |
| 10                         | 0.02                  | 0.04    | 2                                | 0.02                  |
| 15                         | 0.03                  | 0.06    | 5                                | 0.04                  |
| 20                         | 0.03                  | 0.06    | 10                               | 0.06                  |
| 25                         | 0.03                  | 0.06    | 25                               | 0.10                  |
| 50                         | 0.05                  | 0.10    |                                  |                       |
| 100                        | 0.08                  | 0.16    |                                  |                       |

\* Accuracy tolerances for volumetric transfer pipets are given by ASTM standard E969 and Federal Specification NNN-P-395.

† Accuracy tolerances for measuring pipets are given by Federal Specification NNN-P-350 and for serological pipets by Federal Specification NNN-P-375.

**TABLE 11.42** Tolerances of Micropipets (Eppendorf)

| Capacity, $\mu$ L | Accuracy, % | Precision, % | Capacity, $\mu$ L | Accuracy, % | Precision, % |
|-------------------|-------------|--------------|-------------------|-------------|--------------|
| 10                | 1.2         | 0.4          | 100               | 0.5         | 0.2          |
| 40                | 0.6         | 0.2          | 250               | 0.5         | 0.15         |
| 50                | 0.5         | 0.2          | 500               | 0.5         | 0.15         |
| 60                | 0.5         | 0.2          | 600               | 0.5         | 0.15         |
| 70                | 0.5         | 0.2          | 900               | 0.5         | 0.15         |
| 80                | 0.5         | 0.2          | 1000              | 0.5         | 0.15         |

**TABLE 11.43** Buret Accuracy Tolerances

| Capacity, mL | Subdivision, mL | Accuracy, $\pm$ mL           |                            |
|--------------|-----------------|------------------------------|----------------------------|
|              |                 | Class A* and precision grade | Class B and standard grade |
| 10           | 0.05            | 0.02                         | 0.04                       |
| 25           | 0.10            | 0.03                         | 0.06                       |
| 50           | 0.10            | 0.05                         | 0.10                       |
| 100          | 0.20            | 0.10                         | 0.20                       |

\* Class A conforms to specifications in ASTM E694 for standard taper stopcocks and to ASTM E287 for Teflon or polytetrafluoroethylene stopcock plugs. The 10-mL size meets the requirements for ASTM D664.

**TABLE 11.44** Factors for Simplified Computation of Volume

The volume is determined by weighing the water, having a temperature of  $t^{\circ}\text{C}$ , contained or delivered by the apparatus at the same temperature. The weight of water,  $w$  grams, is obtained with brass weights in air having a density of 1.20 mg/mL.

For apparatus made of soft glass, the volume contained or delivered at  $20^{\circ}\text{C}$  is given by

$$\nu_{20} = wf_{20} \text{ mL}$$

where  $\nu_{20}$  is the volume at  $20^{\circ}$  and  $f_{20}$  is the factor (apparent specific volume) obtained from the table below for the temperature  $t$  at which the calibration is performed. The volume at any other temperature  $t'$  may then be obtained from

$$\nu' = \nu_{20}[1 + 0.00002(t' - 20)] \text{ mL}$$

For apparatus made of any other material, the volume contained or delivered at the temperature  $t$  is

$$\nu_t = wf_t \text{ mL}$$

where  $w$  is again the weight in air obtained with brass weights (in grams), and  $f_t$  is the factor given in the third column of the table for the temperature  $t$ . The volume at any temperature  $t'$  may then be obtained from

$$\nu'_t = \nu_t[1 + \beta(t' - t)] \text{ mL}$$

where  $\beta$  is the cubical coefficient of thermal expansion of the material from which the apparatus is made. Approximate values of  $\beta$  for some frequently encountered materials are given in Table 11.45.

| $t, ^{\circ}\text{C}$ | $f_{20}$ | $f_t$    | $t, ^{\circ}\text{C}$ | $f_{20}$ | $f_t$    |
|-----------------------|----------|----------|-----------------------|----------|----------|
| 0                     | 1.001 62 | 1.001 22 | 20                    | 1.002 86 | 1.002 86 |
| 1                     | 54       | 16       | 21                    | 1.003 05 | 1.003 07 |
| 2                     | 48       | 12       | 22                    | 26       | 30       |
| 3                     | 43       | 09       | 23                    | 47       | 53       |
| 4                     | 41       | 09       | 24                    | 69       | 77       |
| 5                     | 1.001 39 | 1.001 09 | 25                    | 1.003 93 | 1.004 03 |
| 6                     | 40       | 12       | 26                    | 1.004 17 | 29       |
| 7                     | 42       | 16       | 27                    | 42       | 56       |
| 8                     | 45       | 21       | 28                    | 68       | 84       |
| 9                     | 50       | 28       | 29                    | 95       | 1.005 13 |
| 10                    | 1.001 56 | 1.001 36 | 30                    | 1.005 23 | 1.005 43 |
| 11                    | 63       | 45       | 31                    | 1.005 52 | 1.005 74 |
| 12                    | 72       | 56       | 32                    | 1.005 82 | 1.006 06 |
| 13                    | 82       | 68       | 33                    | 1.006 13 | 1.006 39 |
| 14                    | 93       | 81       | 34                    | 1.006 44 | 1.006 72 |
| 15                    | 1.002 06 | 1.001 96 | 35                    | 1.006 77 | 1.007 07 |
| 16                    | 20       | 1.002 12 | 36                    | 1.007 10 | 1.007 42 |
| 17                    | 35       | 29       | 37                    | 1.007 44 | 1.007 78 |
| 18                    | 51       | 47       | 38                    | 1.007 79 | 1.008 15 |
| 19                    | 68       | 66       | 39                    | 1.008 15 | 1.008 53 |
|                       |          |          | 40                    | 1.008 52 | 1.008 91 |

**TABLE 11.45** Cubical Coefficients of Thermal Expansion

This table lists values of  $\beta$ , the cubical coefficient of thermal expansion, taken from “Essentials of Quantitative Analysis,” by Benedetti-Pichler, and from various other sources. The value of  $\beta$  represents the relative increases in volume for a change in temperature of 1°C at temperatures in the vicinity of 25°C, and is equal to  $3\alpha$ , where  $\alpha$  is the linear coefficient of thermal expansion. Data are given for the types of glass from which volumetric apparatus is most commonly made, and also for some other materials which have been or may be used in the fabrication of apparatus employed in analytical work.

| Material                            | $\beta$               |
|-------------------------------------|-----------------------|
| <b>Glasses</b>                      |                       |
| Alkali-resistant, Corning 728       | $1.90 \times 10^{-5}$ |
| Gerateglas, Schott G20              | 1.47                  |
| Kimble KG-33 (borosilicate)         | 0.96                  |
| N-51A (“Resistant”)                 | 1.47                  |
| R-6 (soft)                          | 2.79                  |
| Pyrex, Corning 744                  | 0.96                  |
| Vitreous silica                     | 0.15                  |
| Vycor, Corning 790                  | 0.24                  |
| <b>Metals</b>                       |                       |
| Brass                               | ca. 5.5               |
| Copper                              | 5.0                   |
| Gold                                | 4.3                   |
| Monel metal                         | 4.0                   |
| Platinum                            | 2.7                   |
| Silver                              | 5.7                   |
| Stainless steel                     | ca. 5.3               |
| Tantalum                            | ca. 2.0               |
| Tungsten                            | 1.3                   |
| <b>Plastics and other materials</b> |                       |
| Hard rubber                         | $24 \times 10^{-5}$   |
| Polyethylene                        | 45–90                 |
| Polystyrene                         | 18–24                 |
| Porcelain                           | ca. 1.2               |
| Teflon (polytetrafluoroethylene)    | 16.5                  |

**TABLE 11.46** General Solubility Rules for Inorganic Compounds

|                                              |                                                                                                                                                                                                                                                                                                                                           |
|----------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Nitrates                                     | All nitrates are soluble.                                                                                                                                                                                                                                                                                                                 |
| Acetates                                     | All acetates are soluble; silver acetate is moderately soluble.                                                                                                                                                                                                                                                                           |
| Chlorides                                    | All chlorides are soluble except AgCl, PbCl <sub>2</sub> , and Hg <sub>2</sub> Cl <sub>2</sub> . PbCl <sub>2</sub> is soluble in hot water, slightly soluble in cold water.                                                                                                                                                               |
| Sulfates                                     | All sulfates are soluble except barium and lead. Silver, mercury(I), and calcium are only slightly soluble.                                                                                                                                                                                                                               |
| Hydrogen sulfates                            | The hydrogen sulfates are more soluble than the sulfates.                                                                                                                                                                                                                                                                                 |
| Carbonates, phosphates, chromates, silicates | All carbonates, phosphates, chromates, and silicates are insoluble, except those of sodium, potassium, and ammonium. An exception is MgCrO <sub>4</sub> which is soluble.                                                                                                                                                                 |
| Hydroxides                                   | All hydroxides (except lithium, sodium, potassium, cesium, rubidium, and ammonia) are insoluble; Ba(OH) <sub>2</sub> is moderately soluble; Ca(OH) <sub>2</sub> and Sr(OH) <sub>2</sub> are slightly soluble.                                                                                                                             |
| Sulfides                                     | All sulfides (except alkali metals, ammonium, magnesium, calcium, and barium) are insoluble. Aluminum and chromium sulfides are hydrolyzed and precipitate as hydroxides.                                                                                                                                                                 |
| Sodium, potassium, ammonium                  | All sodium, potassium, and ammonium salts are soluble. Exceptions: Na <sub>4</sub> Sb <sub>2</sub> O <sub>7</sub> , K <sub>2</sub> NaCo(NO <sub>2</sub> ) <sub>6</sub> , K <sub>2</sub> PtCl <sub>6</sub> , (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub> , and (NH <sub>4</sub> ) <sub>2</sub> NaCo(NO <sub>2</sub> ) <sub>6</sub> . |
| Silver                                       | All silver salts are insoluble. Exceptions: AgNO <sub>3</sub> and AgClO <sub>4</sub> ; AgC <sub>2</sub> H <sub>3</sub> O <sub>2</sub> and Ag <sub>2</sub> SO <sub>4</sub> are moderately soluble.                                                                                                                                         |

11.7 LABORATORY SOLUTIONS

TABLE 11.47 Concentrations of Commonly Used Acids and Bases

Freshly opened bottles of these reagents are generally of the concentrations indicated in the table. This may not be true of bottles long opened and this is especially true of ammonium hydroxide, which rapidly loses its strength. In preparing volumetric solutions, it is well to be on the safe side and take a little more than the calculated volume of the concentrated reagent, since it is much easier to dilute a concentrated solution than to strengthen one that is too weak.

A concentrated C.P. reagent usually comes to the laboratory in a bottle having a label which states its molecular weight  $w$ , its density (or its specific gravity)  $d$ , and its percentage assay  $p$ . When such a reagent is used to prepare an aqueous solution of desired molarity  $M$ , a convenient formula to employ is

$$V = \frac{100 \text{ } wM}{pd}$$

where  $V$  is the number of milliliters of concentrated reagent required for 1 liter of the dilute solution.

*Example:* Sulfuric acid has the molecular weight 98.08. If the concentrated acid assays 95.5% and has the specific gravity 1.84, the volume required for 1 liter of a 0.1 molar solution is

$$V = \frac{100 \times 98.08 \times 0.1}{95.5 \times 1.84} = 5.58 \text{ mL}$$

| Reagent                                  | Formula Weight | Density, g · mL <sup>-1</sup> (20°C) | Weight % (approx) | Molarity | V, mL* |
|------------------------------------------|----------------|--------------------------------------|-------------------|----------|--------|
| Acetic acid                              | 60.05          | 1.05                                 | 99.8              | 17.45    | 57.3   |
| Ammonium hydroxide (as NH <sub>3</sub> ) | 35.05<br>17.03 | 0.90                                 | 56.6<br>28.0      | 14.53    | 60.0   |
| Ethylenediamine                          | 60.10          | 0.899                                | 100               | 15.0     | 66.7   |
| Formic acid                              | 46.03          | 1.20                                 | 90.5              | 23.6     | 42.5   |
| Hydrazine                                | 32.05          | 1.011                                | 95                | 30.0     | 33.3   |
| Hydriodic acid                           | 127.91         | 1.70                                 | 57                | 7.6      | 132    |
| Hydrobromic acid                         | 80.92          | 1.49                                 | 48                | 8.84     | 113    |
| Hydrochloric acid                        | 36.46          | 1.19                                 | 37.2              | 12.1     | 82.5   |
| Hydrofluoric acid                        | 20.0           | 1.18                                 | 49.0              | 28.9     | 34.5   |
| Nitric acid                              | 63.01          | 1.42                                 | 70.4              | 15.9     | 63.0   |
| Perchloric acid                          | 100.47         | 1.67                                 | 70.5              | 11.7     | 85.5   |
| Phosphoric acid                          | 97.10          | 1.70                                 | 85.5              | 14.8     | 67.5   |
| Pyridine                                 | 79.10          | 0.982                                | 100               | 12.4     | 80.6   |
| Potassium hydroxide (soln)               | 56.11          | 1.46                                 | 45                | 11.7     | 85.5   |
| Sodium hydroxide (soln)                  | 40.00          | 1.54                                 | 50.5              | 19.4     | 51.5   |
| Sulfuric acid                            | 98.08          | 1.84                                 | 96.0              | 18.0     | 55.8   |
| Triethanolamine                          | 149.19         | 1.124                                | 100               | 7.53     | 132.7  |

\* V, mL = volume in milliliters needed to prepare 1 liter of 1 molar solution.

**TABLE 11.48** Standard Stock Solutions\*

| Element    | Procedure                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Aluminum   | Dissolve 1.000 g Al wire in minimum amount of 2 M HCl; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Antimony   | Dissolve 1.000 g Sb in (1) 10 ml HNO <sub>3</sub> plus 5 ml HCl, and dilute to volume when dissolution is complete; or (2) 18 ml HBr plus 2 ml liquid Br <sub>2</sub> ; when dissolution is complete add 10 ml HClO <sub>4</sub> , heat in a well-ventilated hood while swirling until white fumes appear and continue for several minutes to expel all HBr, then cool and dilute to volume.                                                                                                                                                                                              |
| Arsenic    | Dissolve 1.3203 g of As <sub>2</sub> O <sub>3</sub> in 3 ml 8 M HCl and dilute to volume; or treat the oxide with 2 g NaOH and 20 ml water; after dissolution dilute to 200 ml, neutralize with HCl (pH meter), and dilute to volume.                                                                                                                                                                                                                                                                                                                                                     |
| Barium     | (1) Dissolve 1.7787 g BaCl <sub>2</sub> · 2H <sub>2</sub> O (fresh crystals) in water and dilute to volume. (2) Dissolve 1.516 g BaCl <sub>2</sub> (dried at 250°C for 2 hr) in water and dilute to volume. (3) Treat 1.4367 g BaCO <sub>3</sub> with 300 ml water, slowly add 10 ml of HCl and, after the CO <sub>2</sub> is released by swirling, dilute to volume.                                                                                                                                                                                                                     |
| Beryllium  | (1) Dissolve 19.655 g BeSO <sub>4</sub> · 4H <sub>2</sub> O in water, add 5 ml HCl (or HNO <sub>3</sub> ), and dilute to volume. (2) Dissolve 1.000 g Be in 25 ml 2 M HCl, then dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                         |
| Bismuth    | Dissolve 1.000 g Bi in 8 ml of 10 M HNO <sub>3</sub> , boil gently to expel brown fumes, and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Boron      | Dissolve 5.720 g fresh crystals of H <sub>3</sub> BO <sub>3</sub> and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Bromine    | Dissolve 1.489 g KBr (or 1.288 g NaBr) in water and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| Cadmium    | (1) Dissolve 1.000 g Cd in 10 ml of 2 M HCl; dilute to volume. (2) Dissolve 2.282 g 3CdSO <sub>4</sub> · 8H <sub>2</sub> O in water; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Calcium    | Place 2.4973 g CaCO <sub>3</sub> in volumetric flask with 300 ml water, carefully add 10 ml HCl; after CO <sub>2</sub> is released by swirling, dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Cerium     | (1) Dissolve 4.515 g (NH <sub>4</sub> ) <sub>4</sub> Ce(SO <sub>4</sub> ) <sub>4</sub> · 2H <sub>2</sub> O in 500 ml water to which 30 ml H <sub>2</sub> SO <sub>4</sub> had been added, cool, and dilute to volume. Advisable to standardize against As <sub>2</sub> O <sub>3</sub> . (2) Dissolve 3.913 g (NH <sub>4</sub> ) <sub>2</sub> Ce(NO <sub>3</sub> ) <sub>6</sub> in 10 ml H <sub>2</sub> SO <sub>4</sub> , stir 2 min, cautiously introduce 15 ml water and again stir 2 min. Repeat addition of water and stirring until all the salt has dissolved, then dilute to volume. |
| Cesium     | Dissolve 1.267 g CsCl and dilute to volume. Standardize: Pipette 25 ml of final solution to Pt dish, add 1 drop H <sub>2</sub> SO <sub>4</sub> , evaporate to dryness, and heat to constant weight at > 800°C. Cs (in µg/ml) = (40)(0.734)(wt of residue)                                                                                                                                                                                                                                                                                                                                 |
| Chlorine   | Dissolve 1.648 g NaCl and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Chromium   | (1) Dissolve 2.829 g K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> in water and dilute to volume. (2) Dissolve 1.000 g Cr in 10 ml HCl, and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Cobalt     | Dissolve 1.000 g Co in 10 ml of 2 M HCl, and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Copper     | (1) Dissolve 3.929 g fresh crystals of CuSO <sub>4</sub> · 5H <sub>2</sub> O, and dilute to volume. (2) Dissolve 1.000 g Cu in 10 ml HCl plus 5 ml water to which HNO <sub>3</sub> (or 30%H <sub>2</sub> O <sub>2</sub> ) is added dropwise until dissolution is complete. Boil to expel oxides of nitrogen and chlorine, then dilute to volume.                                                                                                                                                                                                                                          |
| Dysprosium | Dissolve 1.1477 g Dy <sub>2</sub> O <sub>3</sub> in 50 ml of 2 M HCl; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Erbium     | Dissolve 1.1436 g Er <sub>2</sub> O <sub>3</sub> in 50 ml of 2 M HCl; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Europium   | Dissolve 1.1579 g Eu <sub>2</sub> O <sub>3</sub> in 50 ml of 2 M HCl; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Fluorine   | Dissolve 2.210 g NaF in water and dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Gadolinium | Dissolve 1.152 g Gd <sub>2</sub> O <sub>3</sub> in 50 ml of 2 M HCl; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Gallium    | Dissolve 1.000 g Ga in 50 ml of 2 M HCl; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| Germanium  | Dissolve 1.4408 g GeO <sub>2</sub> with 50 g oxalic acid in 100 ml of water; dilute to volume.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

\* 1000 µg/mL as the element in a final volume of 1 liter unless stated otherwise.

From J. A. Dean and T. C. Rains, "Standard Solutions for Flame Spectrometry," in *Flame Emission and Atomic Absorption Spectrometry*, J. A. Dean and T. C. Rains (Eds.), Vol. 2, Chap. 13, Marcel Dekker, New York, 1971.

**TABLE 11.48** Standard Stock Solutions (*Continued*)

| Element      | Procedure                                                                                                                                                                                                                                                                                                                                                                                                           |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Gold         | Dissolve 1.000 g Au in 10 ml of hot $\text{HNO}_3$ by dropwise addition of $\text{HCl}$ , boil to expel oxides of nitrogen and chlorine, and dilute to volume. Store in amber container away from light.                                                                                                                                                                                                            |
| Hafnium      | Transfer 1.000 g Hf to Pt dish, add 10 ml of 9 M $\text{H}_2\text{SO}_4$ , and then slowly add $\text{HF}$ dropwise until dissolution is complete. Dilute to volume with 10% $\text{H}_2\text{SO}_4$ .                                                                                                                                                                                                              |
| Holmium      | Dissolve 1.1455 g $\text{Ho}_2\text{O}_3$ in 50 ml of 2 M $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                          |
| Indium       | Dissolve 1.000 g In in 50 ml of 2 M $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                                                |
| Iodine       | Dissolve 1.308 g $\text{KI}$ in water and dilute to volume.                                                                                                                                                                                                                                                                                                                                                         |
| Iridium      | (1) Dissolve 2.465 g $\text{Na}_3\text{IrCl}_6$ in water and dilute to volume. (2) Transfer 1.000 g Ir sponge to a glass tube, add 20 ml of $\text{HCl}$ and 1 ml of $\text{HClO}_4$ . Seal the tube and place in an oven at $300^\circ\text{C}$ for 24 hr. Cool, break open the tube, transfer the solution to a volumetric flask, and dilute to volume. Observe all safety precautions in opening the glass tube. |
| Iron         | Dissolve 1.000 g Fe wire in 20 ml of 5 M $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                                           |
| Lanthanum    | Dissolve 1.1717 g $\text{La}_2\text{O}_3$ (dried at $110^\circ\text{C}$ ) in 50 ml of 5 M $\text{HCl}$ , and dilute to volume.                                                                                                                                                                                                                                                                                      |
| Lead         | (1) Dissolve 1.5985 g $\text{Pb}(\text{NO}_3)_2$ in water plus 10 ml $\text{HNO}_3$ , and dilute to volume. (2) Dissolve 1.000 g Pb in 10 ml $\text{HNO}_3$ , and dilute to volume.                                                                                                                                                                                                                                 |
| Lithium      | Dissolve a slurry of 5.3228 g $\text{Li}_2\text{CO}_3$ in 300 ml of water by addition of 15 ml $\text{HCl}$ ; after release of $\text{CO}_2$ by swirling, dilute to volume.                                                                                                                                                                                                                                         |
| Lutetium     | Dissolve 1.6079 g $\text{LuCl}_3$ in water and dilute to volume.                                                                                                                                                                                                                                                                                                                                                    |
| Magnesium    | Dissolve 1.000 g Mg in 50 ml of 1 M $\text{HCl}$ and dilute to volume.                                                                                                                                                                                                                                                                                                                                              |
| Manganese    | (1) Dissolve 1.000 g Mn in 10 ml $\text{HCl}$ plus 1 ml $\text{HNO}_3$ , and dilute to volume. (2) Dissolve 3.0764 g $\text{MnSO}_4 \cdot \text{H}_2\text{O}$ (dried at $105^\circ\text{C}$ for 4 hr) in water and dilute to volume. (3) Dissolve 1.5824 g $\text{MnO}_2$ in 10 $\text{HCl}$ in a good hood, evaporate to gentle dryness, dissolve residue in water and dilute to volume.                           |
| Mercury      | Dissolve 1.000 g Hg in 10 ml of 5 M $\text{HNO}_3$ and dilute to volume.                                                                                                                                                                                                                                                                                                                                            |
| Molybdenum   | (1) Dissolve 2.0425 g $(\text{NH}_4)_2\text{MoO}_4$ in water and dilute to volume. (2) Dissolve 1.5003 g $\text{MoO}_3$ in 100 ml of 2 M ammonia, and dilute to volume.                                                                                                                                                                                                                                             |
| Neodymium    | Dissolve 1.7373 g $\text{NdCl}_3$ in 100 ml 1 M $\text{HCl}$ and dilute to volume.                                                                                                                                                                                                                                                                                                                                  |
| Nickel       | Dissolve 1.000 g Ni in 10 ml hot $\text{HNO}_3$ , cool, and dilute to volume.                                                                                                                                                                                                                                                                                                                                       |
| Niobium      | Transfer 1.000 g Nb (or 1.4305 g $\text{Nb}_2\text{O}_5$ ) to Pt dish, add 20 ml $\text{HF}$ , and heat gently to complete dissolution. Cool, add 40 ml $\text{H}_2\text{SO}_4$ , and evaporate to fumes of $\text{SO}_3$ . Cool and dilute to volume with 8 M $\text{H}_2\text{SO}_4$ .                                                                                                                            |
| Osmium       | Dissolve 1.3360 g $\text{OsO}_4$ in water and dilute to 100 ml. Prepare only as needed as solution loses strength on standing unless Os is reduced by $\text{SO}_2$ and water is replaced by 100 ml 0.1 M $\text{HCl}$ .                                                                                                                                                                                            |
| Palladium    | Dissolve 1.000 g Pd in 10 ml of $\text{HNO}_3$ by dropwise addition of $\text{HCl}$ to hot solution; dilute to volume.                                                                                                                                                                                                                                                                                              |
| Phosphorus   | Dissolve 4.260 g $(\text{NH}_4)_2\text{HPO}_4$ in water and dilute to volume.                                                                                                                                                                                                                                                                                                                                       |
| Platinum     | Dissolve 1.000 g Pt in 40 ml of hot aqua regia, evaporate to incipient dryness, add 10 ml $\text{HCl}$ and again evaporate to moist residue. Add 10 ml $\text{HCl}$ and dilute to volume.                                                                                                                                                                                                                           |
| Potassium    | Dissolve 1.9067 g $\text{KCl}$ (or 2.8415 g $\text{KNO}_3$ ) in water and dilute to volume.                                                                                                                                                                                                                                                                                                                         |
| Praseodymium | Dissolve 1.1703 g $\text{Pr}_2\text{O}_3$ in 50 ml of 2 M $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                          |
| Rhenium      | Dissolve 1.000 g Re in 10 ml of 8 M $\text{HNO}_3$ in an ice bath until initial reaction subsides, then dilute to volume.                                                                                                                                                                                                                                                                                           |
| Rhodium      | Dissolve 1.000 g Rh by the sealed-tube method described under iridium.                                                                                                                                                                                                                                                                                                                                              |
| Rubidium     | Dissolve 1.4148 g $\text{RbCl}$ in water. Standardize as described under cesium. $\text{Rb}$ (in $\mu\text{g}/\text{ml}$ ) = $(40)(0.320)/(\text{wt of residue})$ .                                                                                                                                                                                                                                                 |
| Ruthenium    | Dissolve 1.317 g $\text{RuO}_2$ in 15 ml of $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                                        |
| Samarium     | Dissolve 1.1596 g $\text{Sm}_2\text{O}_3$ in 50 ml of 2 M $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                          |
| Scandium     | Dissolve 1.5338 g $\text{Sc}_2\text{O}_3$ in 50 ml of 2 M $\text{HCl}$ ; dilute to volume.                                                                                                                                                                                                                                                                                                                          |

**TABLE 11.48** Standard Stock Solutions (*Continued*)

| Element   | Procedure                                                                                                                                                                                                                                                                                    |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Selenium  | Dissolve 1.4050 g $\text{SeO}_2$ in water and dilute to volume or dissolve 1.000 g Se in 5 ml of $\text{HNO}_3$ , then dilute to volume.                                                                                                                                                     |
| Silicon   | Fuse 2.1393 g $\text{SiO}_2$ with 4.60 g $\text{Na}_2\text{CO}_3$ , maintaining melt for 15 min in Pt crucible. Cool, dissolve in warm water, and dilute to volume. Solution contains also 2000 $\mu\text{g}/\text{ml}$ sodium.                                                              |
| Silver    | (1) Dissolve 1.5748 g $\text{AgNO}_3$ in water and dilute to volume. (2) Dissolve 1.000 g Ag in 10 ml of $\text{HNO}_3$ ; dilute to volume. Store in amber glass container away from light.                                                                                                  |
| Sodium    | Dissolve 2.5421 g NaCl in water and dilute to volume.                                                                                                                                                                                                                                        |
| Strontium | Dissolve a slurry of 1.6849 g $\text{SrCO}_3$ in 300 ml of water by careful addition of 10 ml of HCl; after release of $\text{CO}_2$ by swirling, dilute to volume.                                                                                                                          |
| Sulfur    | Dissolve 4.122 g $(\text{NH}_4)_2\text{SO}_4$ in water and dilute to volume.                                                                                                                                                                                                                 |
| Tantalum  | Transfer 1.000 g Ta (or 1.2210 g $\text{Ta}_2\text{O}_5$ ) to Pt dish, add 20 ml of HF, and heat gently to complete the dissolution. Cool, add 40 ml of $\text{H}_2\text{SO}_4$ and evaporate to heavy fumes of $\text{SO}_3$ . Cool and dilute to volume with 50% $\text{H}_2\text{SO}_4$ . |
| Tellurium | (1) Dissolve 1.2508 g $\text{TeO}_2$ in 10 ml of HCl; dilute to volume. (2) Dissolve 1.000 g Te in 10 ml of warm HCl with dropwise addition of $\text{HNO}_3$ , then dilute to volume.                                                                                                       |
| Terbium   | Dissolve 1.6692 g of $\text{TbCl}_3$ in water, add 1 ml of HCl, and dilute to volume.                                                                                                                                                                                                        |
| Thallium  | Dissolve 1.3034 g $\text{TlNO}_3$ in water and dilute to volume.                                                                                                                                                                                                                             |
| Thorium   | Dissolve 2.3794 g $\text{Th}(\text{NO}_3)_4 \cdot 4\text{H}_2\text{O}$ in water, add 5 ml $\text{HNO}_3$ , and dilute to volume.                                                                                                                                                             |
| Thulium   | Dissolve 1.142 g $\text{Tm}_2\text{O}_3$ in 50 ml of 2 M HCl; dilute to volume.                                                                                                                                                                                                              |
| Tin       | Dissolve 1.000 g Sn in 15 ml of warm HCl; dilute to volume.                                                                                                                                                                                                                                  |
| Titanium  | Dissolve 1.000 g Ti in 10 ml of $\text{H}_2\text{SO}_4$ with dropwise addition of $\text{HNO}_3$ ; dilute to volume with 5% $\text{H}_2\text{SO}_4$ .                                                                                                                                        |
| Tungsten  | Dissolve 1.7941 g of $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$ in water and dilute to volume.                                                                                                                                                                                       |
| Uranium   | Dissolve 2.1095 g $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (or 1.7734 g uranyl acetate dihydrate) in water and dilute to volume.                                                                                                                                               |
| Vanadium  | Dissolve 2.2963 g $\text{NH}_4\text{VO}_3$ in 100 ml of water plus 10 ml of $\text{HNO}_3$ ; dilute to volume.                                                                                                                                                                               |
| Ytterbium | Dissolve 1.6147 g $\text{YbCl}_3$ in water and dilute to volume.                                                                                                                                                                                                                             |
| Yttrium   | Dissolve 1.2692 g $\text{Y}_2\text{O}_3$ in 50 ml of 2 M HCl and dilute to volume.                                                                                                                                                                                                           |
| Zinc      | Dissolve 1.000 g Zn in 10 ml of HCl; dilute to volume.                                                                                                                                                                                                                                       |
| Zirconium | Dissolve 3.533 g $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$ in 50 ml of 2 M HCl, and dilute to volume. Solution should be standardized.                                                                                                                                                      |

### 11.7.1 General Reagents, Indicators, and Special Solutions

Unless otherwise stated, the term *g per liter* signifies grams of the formula indicated dissolved in water and made up to a liter of solution.

**Acetic acid**,  $\text{HC}_2\text{H}_3\text{O}_2$ —6N: 350 mL glacial acetic acid per liter.

**Alcohol, amyl**,  $\text{C}_5\text{H}_{11}\text{OH}$ : use as purchased.

**Alcohol, ethyl**,  $\text{C}_2\text{H}_5\text{OH}$ ; 95% alcohol, as purchased.

**Alizarin**, dihydroxyanthraquinone (indicator): dissolve 0.1 g in 100 mL alcohol; pH range yellow 5.5–6.8 red.

**Alizarin yellow R**, sodium *p*-nitrobenzeneazosalicylate (indicator): dissolve 0.1 g in 100 mL water; pH range yellow 10.1–violet 12.1.



**Alizarin yellow GG**, salicyl yellow, sodium *m*-nitrobenzeneazosalicylate (indicator): dissolve 0.1 g in 100 mL 50% alcohol; pH range yellow 10.0–12.0 lilac.

**Alizarin S**, alizarin carmine, sodium alizarin sulfonate (indicator): dissolve 0.1 g in 100 mL water; pH range yellow 3.7–5.2 violet.

**Aluminon** (qualitative test for aluminum). The reagent consists of 0.1% solution of the ammonium salt of aurin tricarboxylic acid. A bright red precipitate, persisting in alkaline solution, indicates aluminum.

**Aluminum chloride**,  $\text{AlCl}_3$ —0.5*N*: 22 g per liter.

**Aluminum nitrate**,  $\text{Al}(\text{NO}_3)_3 \cdot 7.5\text{H}_2\text{O}$ —0.5*N*: 58 g per liter.

**Aluminum sulfate**,  $\text{Al}_2(\text{SO}_4)_3 \cdot 18\text{H}_2\text{O}$ —0.5*N*: 55 g per liter.

**Ammonium acetate**,  $\text{NH}_4\text{C}_2\text{H}_3\text{O}_2$ —3*N*: 231 g per liter.

**Ammonium carbonate**,  $(\text{NH}_4)_2\text{CO}_3 \cdot \text{H}_2\text{O}$ —3*N*: 171 g per liter; for the anhydrous salt: 144 g per liter.

**Ammonium chloride**,  $\text{NH}_4\text{Cl}$ —3*N*: 161 g per liter.

**Ammonium hydroxide**,  $\text{NH}_4\text{OH}$ —15*N*: the concentrated solution which contains 28%  $\text{NH}_3$ ; for 6*N*: 400 mL per liter.

**Ammonium molybdate**,  $(\text{NH}_4)_2\text{MoO}_4$ —*N*: dissolve 88.3 g of solid  $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$  in 100 mL 6*N*  $\text{NH}_4\text{OH}$ . Add 240 g of solid  $\text{NH}_4\text{NO}_3$  and dilute to 1 liter. Another method is to take 72 g of  $\text{MoO}_3$ , add 130 mL of water and 75 mL of 15*N*  $\text{NH}_4\text{OH}$ ; stir mechanically until nearly all has dissolved, then add it to a solution of 240 mL concentrated  $\text{HNO}_3$  and 500 mL of water; stir continuously while solutions are being mixed; allow to stand 3 days, filter, and use the clear filtrate.

**Ammonium nitrate**,  $\text{NH}_4\text{NO}_3$ —*N*: 80 g per liter.

**Ammonium oxalate**,  $(\text{NH}_4)_2\text{C}_2\text{O}_4 \cdot \text{H}_2\text{O}$ —0.5*N*: 40 g per liter.

**Ammonium polysulfide** (yellow ammonium sulfide),  $(\text{NH}_4)_2\text{S}_x$ : allow the colorless  $(\text{NH}_4)_2\text{S}$  to stand, or add sulfur.

**Ammonium sulfate**,  $(\text{NH}_4)_2\text{SO}_4$ —0.5*N*: 33 g per liter; saturated: dissolve 780 g of  $(\text{NH}_4)_2\text{SO}_4$  in water and make up to a liter.

**Ammonium sulfide** (colorless),  $(\text{NH}_4)_2\text{S}$ —saturated: pass  $\text{H}_2\text{S}$  through 200 mL of concentrated  $\text{NH}_4\text{OH}$  in the cold until no more gas is dissolved, add 200 mL  $\text{NH}_4\text{OH}$  and dilute with water to a liter; the addition of 15 g of sulfur is sufficient to make the polysulfide.

**Antimony pentachloride**,  $\text{SbCl}_5$ —0.5*N*: 39 g per liter.

**Antimony trichloride**,  $\text{SbCl}_3$ —0.5*N*: 38 g per liter.

**Aqua regia**: mix 3 parts of concentrated  $\text{HCl}$  and 1 part of concentrated  $\text{HNO}_3$  just before ready to use.

**Arsenic acid**,  $\text{H}_3\text{AsO}_4 \cdot 0.5\text{H}_2\text{O}$ —0.5*N* ( $= \frac{1}{2}\text{H}_3\text{AsO}_4 \div 5$ ): 15 g per liter.

**Arsenous oxide**,  $\text{As}_2\text{O}_3$ —0.25*N*: 8 g per liter for saturation.

**Aurichloric acid**,  $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$ : dissolve in ten parts of water.

**Aurin**, *see* rosolic acid.

**Azolitmin solution** (indicator); make up a 1% solution of azolitmin by boiling in water for 5 minutes; it may be necessary to add a small amount of  $\text{NaOH}$  to make the solution neutral; pH range red 4.5–8.3 blue.

**Bang's reagent** (for glucose estimation): dissolve 100 g of  $\text{K}_2\text{CO}_3$ , 66 g of KCl, and 160 of  $\text{KHCO}_3$  in the order given in about 700 mL of water at  $30^\circ\text{C}$ . Add 4.4 g of copper sulfate and dilute to 1 liter after the  $\text{CO}_2$  is evolved. This solution should be shaken only in such a manner as not to allow the entry of air. After 24 hours 300 mL diluted to a liter with saturated KCl solution, shaken gently and used after 24 hours; 50 mL  $\equiv$  10 mg glucose.

**Barfoed's reagent** (test for glucose): dissolve 66 g of cupric acetate and 10 mL of glacial acetic acid in water and dilute to 1 liter.

**Barium chloride**,  $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$ —0.5*N*: 61 g per liter.

**Barium hydroxide**,  $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ —0.2*N*: 32 g per liter for saturation.

**Barium nitrate**,  $\text{Ba}(\text{NO}_3)_2$ —0.5*N*: 65 g per liter.

**Baudisch's reagent**: see cupferron.

**Benedict's qualitative reagent** (for glucose): dissolve 173 g of sodium citrate and 100 g of anhydrous sodium carbonate in about 600 mL of water, and dilute to 850 mL; dissolve 17.3 g of  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  in 100 mL of water and dilute to 150 mL; this solution is added to the citrate-carbonate solution with constant stirring. See also the quantitative reagent below.

**Benedict's quantitative reagent** (sugar in urine): This solution contains 18 g copper sulfate, 100 g of anhydrous sodium carbonate, 200 g of potassium citrate, 125 g of potassium thiocyanate, and 0.25 g of potassium ferrocyanide per liter; 1 mL of this solution  $\equiv$  0.002 g sugar.

**Benzidine hydrochloride solution** (for sulfate determination): mix 6.7 g of benzidine [ $\text{C}_{12}\text{H}_8(\text{NH}_2)_2$ ] or 8.0 g of the hydrochloride [ $\text{C}_{12}\text{H}_8(\text{NH}_2)_2 \cdot 2\text{HCl}$ ] into a paste with 20 mL of water; add 20 mL of HCl (sp. gr. 1.12) and dilute the mixture to 1 liter with water; each mL of this solution is equivalent to 0.00357 g  $\text{H}_2\text{SO}_4$ .

**Benzopurpurine 4B** (indicator): dissolve 0.1 g in 100 mL water; pH range blue-violet 1.3–4.0 red.

**Benzoyl auramine** (indicator): dissolve 0.25 g in 100 mL methyl alcohol; pH range violet 5.0–5.6 pale yellow. Since this compound is not stable in aqueous solution, hydrolyzing slowly in neutral medium, more rapidly in alkaline, and still more rapidly in acid solution, the indicator should not be added until one is ready to titrate. The acid quinoid form of the compound is dichroic, showing a red-violet in thick layers and blue in thin. At a pH of 5.4 the indicator appears a neutral gray color by daylight or a pale red under tungsten light. The change to yellow is easily recognized in either case. Cf. Scanlan and Reid, *Ind. Eng. Chem., Anal. Ed.* 7:125 (1935).

**Bertrand's reagents** (glucose estimation): (a) 40 g of copper sulfate diluted to 1 liter; (b) rochelle salt 200 g, NaOH 150 g, and sufficient water to make 1 liter; (c) ferric sulfate 50 g,  $\text{H}_2\text{SO}_4$  200 g, and sufficient water to make 1 liter; (d)  $\text{KMnO}_4$  5 g and sufficient water to make 1 liter.

**Bial's reagent** (for pentoses): dissolve 1 g of orcinol in 500 mL of 30% HCl to which 30 drops of a 10% ferric chloride solution have been added.

**Bismuth chloride**,  $\text{BiCl}_3$ —0.5*N*: 52 g per liter, using 1:5 HCl in place of water.

**Bismuth nitrate**,  $\text{Bi}(\text{N}_2\text{O}_5)_3 \cdot 5\text{H}_2\text{O}$ —0.25*N*: 40 g per liter, using 1:5  $\text{HNO}_3$  in place of water.

**Bismuth standard solution** (quantitative color test for Bi): dissolve 1 g of bismuth in a mixture of 3 mL of concentrated  $\text{HNO}_3$  and 2.8 mL of  $\text{H}_2\text{O}$  and make up to 100 mL with glycerol. Also dissolve 5 g of KI in 5 mL of water and make up to 100 mL with glycerol. The two solutions are used together in the colorimetric estimation of Bi.

**Boutron-Boudet solution**: see soap solution.

**Bromchlorophenol blue**, dibromodichlorophenol-sulfonphthalein (indicator): dissolve 0.1 g in 8.6 mL 0.02 *N* NaOH and dilute with water to 250 mL; pH range yellow 3.2–4.8 blue.

**Bromcresol green**, tetrabromo-*m*-cresol-sulfonphthalein (indicator): dissolve 0.1 g in 7.15 mL 0.02 *N* NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL 20% alcohol; pH range yellow 4.0–5.6 blue.

**Bromcresol purple**, dibromo-*o*-cresol-sulfonphthalein (indicator): dissolve 0.1 g in 9.5 mL 0.02 *N* NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL 20% alcohol; pH range yellow 5.2–6.8 purple.

**Bromine water**, saturated solution: to 400 mL water add 20 mL of bromine; use a glass stopper coated with petrolatum.

**Bromphenol blue**, tetrabromophenol-sulfonphthalein (indicator): dissolve 0.1 g in 7.45 mL 0.02 *N* NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL 20% alcohol; pH range yellow 3.6–4.6 violet-blue.

**Bromphenol red**, dibromophenol-sulfonphthalein (indicator): dissolve 0.1 g in 9.75 mL 0.02 *N* NaOH and dilute with water to 250 mL; pH range yellow 5.2–7.0 red.

**Bromthymol blue**, dibromothymol-sulfonphthalein (indicator): dissolve 0.1 g in 8.0 mL 0.02 *N* NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL of 20% alcohol; pH range yellow 6.0–7.6 blue.

**Brucke's reagent** (protein precipitant): dissolve 50 g of KI in 500 mL of water, saturate with HgI<sub>2</sub> (about 120 g), and dilute to 1 liter.

**Cadmium chloride**, CdCl<sub>2</sub>—0.5*N*: 46 g per liter.

**Cadmium nitrate**, Cd(NO<sub>3</sub>)<sub>2</sub> · 4H<sub>2</sub>O—0.5*N*: 77 g per liter.

**Cadmium sulfate**, CdSO<sub>4</sub> · 4H<sub>2</sub>O—0.5*N*: 70 g per liter.

**Calcium chloride**, CaCl<sub>2</sub> · 6H<sub>2</sub>O—0.5*N*: 55 g per liter.

**Calcium hydroxide**, Ca(OH)<sub>2</sub>—0.04*N*: 10 g per liter for saturation.

**Calcium nitrate**, Ca(NO<sub>3</sub>)<sub>2</sub> · 4H<sub>2</sub>O—0.5*N*: 59 g per liter.

**Calcium sulfate**, CaSO<sub>4</sub> · 2H<sub>2</sub>O—0.03*N*: mechanically stir 10 g in a liter of water for 3 hours; decant and use the clear liquid.

**Carbon disulfide**, CS<sub>2</sub>: commercial grade which is colorless.

**Chloride reagent**: dissolve 1.7 g of AgNO<sub>3</sub> and 25 g KNO<sub>3</sub> in water, add 17 mL of concentrated NH<sub>4</sub>OH and make up to 1 liter with water.

**Chlorine water**, saturated solution: pass chlorine gas into small amounts of water as needed; solutions deteriorate on standing.

**Chloroform**, CHCl<sub>3</sub>: commercial grade.

**Chloroplatinic acid**, H<sub>2</sub>PtCl<sub>6</sub> · 6H<sub>2</sub>O—10% solution: dissolve 1 g in 9 mL of water; keep in a dropping bottle.

**Chlorphenol red**, dichlorophenol-sulfonphthalein (indicator): dissolve 0.1 g in 11.8 mL 0.02 *N* NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL 20% alcohol; pH range yellow 5.2–6.6 red.

**Chromic chloride**, CrCl<sub>3</sub>—0.5*N*: 26 g per liter.

**Chromic nitrate**, Cr(NO<sub>3</sub>)<sub>3</sub>—0.5*N*: 40 g per liter.

**Chromic sulfate**, Cr<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> · 18H<sub>2</sub>O—0.5*N*: 60 g per liter.

**Cobaltous nitrate**, Co(NO<sub>3</sub>)<sub>2</sub> · 6H<sub>2</sub>O—0.5*N*: 73 g per liter.

**Cobaltous sulfate**,  $\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$ —0.5*N*: 70 g per liter.

**Cochineal** (indicator): triturate 1 g with 75 mL alcohol and 75 mL water, let stand for two days and filter; pH range red 4.8–6.2 violet.

**Congo red**, sodium tetrazodiphenyl-naphthionate (indicator): dissolve 0.1 g in 100 mL water; pH range blue 3.0–5.2 red.

**Corallin** (indicator): *see* rosolic acid.

**Cresol red**, *o*-cresol-sulfonphthalein (indicator): dissolve 0.1 g in 13.1 mL 0.02*N* NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL 20% alcohol; pH range yellow 7.2–8.8 red.

***o*-Cresolphthalein** (indicator): dissolve 0.1 g in 250 mL alcohol; pH range colorless 8.2–10.4 red.

**Cupferron** (iron analysis): dissolve 6 g of ammonium nitrosophenyl-hydroxylamine (cupferron) in water and dilute to 100 mL. This solution is stable for about one week if protected from light.

**Cupric chloride**,  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ —0.5*N*: 43 g per liter.

**Cupric nitrate**,  $\text{Cu}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ —0.5*N*: 74 g per liter.

**Cupric sulfate**,  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ —0.5*N*: 62 g per liter.

**Cuprous chloride**,  $\text{CuCl}$ —0.5*N*: 50 g per liter, using 1:5 HCl in place of water.

**Cuprous chloride**, acid (for gas analysis, absorption of CO): cover the bottom of a 2-liter bottle with a layer of copper oxide  $\frac{3}{8}$  inch deep, and place a bundle of copper wire an inch thick in the bottle so that it extends from the top to the bottom. Fill the bottle with HCl (sp. gr. 1.10). The bottle is shaken occasionally, and when the solution is colorless or nearly so, it is poured into half-liter bottles containing copper wire. The large bottle may be filled with hydrochloric acid, and by adding the oxide or wire when either is exhausted, a constant supply of the reagent is available.

**Cuprous chloride, ammoniacal**: this solution is used for the same purpose and is made in the same manner as the acid cuprous chloride above, except that the acid solution is treated with ammonia until a faint odor of ammonia is perceptible. Copper wire should be kept with the solution as in the acid reagent.

**Curcumin** (indicator): prepare a saturated aqueous solution; pH range yellow 6.0–8.0 brownish red.

**Dibromophenol-tetrabromophenol-sulfonphthalein** (indicator): dissolve 0.1 g in 1.21 mL 0.1*N* NaOH and dilute with water to 250 mL; pH range yellow 5.6–7.2 purple.

**Dimethyl glyoxime**,  $(\text{CH}_3\text{CNOH})_2$ —0.01*N*: 6 g in 500 mL of 95% alcohol.

**2,4-Dinitrophenol** (indicator): dissolve 0.1 g in a few mL alcohol, then dilute with water to 100 mL; pH range colorless 2.6–4.0 yellow.

**2,5-Dinitrophenol** (indicator): dissolve 0.1 g in 20 mL alcohol, then dilute with water to 100 mL; pH range colorless 4–5.8 yellow.

**2,6-Dinitrophenol** (indicator): dissolve 0.1 g in a few mL alcohol, then dilute with water to 100 mL; pH range colorless 2.4–4.0 yellow.

**Esbach's reagent** (estimation of proteins): dissolve 10 g of picric acid and 20 g of citric acid in water and dilute to 1 liter.

**Eschka's mixture** (sulfur in coal): mix 2 parts of porous calcined MgO with 1 part of anhydrous  $\text{Na}_2\text{CO}_3$ ; not a solution but a dry mixture.

**Ether**,  $(\text{C}_2\text{H}_5)_2\text{O}$ —use commercial grade.

***p*-Ethoxychrysoidine**, *p*-ethoxybenzeneazo-*m*-phenylenediamine (indicator): dissolve 0.1 g of the base in 100 mL 90% alcohol; or, 0.1 g of the hydrochloride salt in 100 mL water; pH range red 3.5–5.5 yellow.

**Ethyl bis-(2,4-dinitrophenyl) acetate** (indicator): the stock solution is prepared by saturating a solution containing equal volumes of alcohol and acetone with the indicator; pH range colorless 7.4–9.1 deep blue. This compound is available commercially. The preparation of this compound is described by Fehnel and Amstutz, *Ind. Eng. Chem., Anal. Ed.* **16**:53 (1944), and by von Richter, *Ber.* **21**:2470 (1888), who recommended it for the titration of orange- and red-colored solutions or dark oils in which the endpoint of phenol-phthalein is not easily visible. The indicator is an orange solid which after crystallization from benzene gives pale yellow crystals melting at 150–153.5°C, uncorrected.

**Fehling's solution** (sugar detection and estimation): (a) Copper sulfate solution: dissolve 34.639 g of  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  in water and dilute to 500 mL. (b) Alkaline tartrate solution: dissolve 173 g of rochelle salts ( $\text{KNaC}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$ ) and 125 g of KOH in water and dilute to 500 mL. Equal volumes of the two solutions are mixed just prior to use. The Methods of the Assoc. of Official Agricultural Chemists give 50 g of NaOH in place of the 125 g KOH.

**Ferric chloride**,  $\text{FeCl}_3$ —0.5*N*: 27 g per liter.

**Ferric nitrate**,  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ —0.5*N*: 67 g per liter.

**Ferrous ammonium sulfate**, Mohr's salt,  $\text{FeSO}_4 \cdot (\text{NH}_4)_2\text{SO}_4 \cdot 6\text{H}_2\text{O}$ —0.5*N*: 196 g per liter.

**Ferrous sulfate**,  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ —0.5*N*: 80 g per liter; add a few drops of  $\text{H}_2\text{SO}_4$ .

**Folin's mixture** (for uric acid): dissolve 500 g of ammonium sulfate, 5 g of uranium acetate, and 6 mL of glacial acetic acid, in 650 mL of water. The volume is about a liter.

**Formal or Formalin**: use the commercial 40% solution of formaldehyde.

**Froehde's reagent** (gives characteristic colorations with certain alkaloids and glycosides): dissolve 0.01 g of sodium molybdate in 1 mL of concentrated  $\text{H}_2\text{SO}_4$ ; use only a freshly prepared solution.

**Gallein** (indicator): dissolve 0.1 g in 100 mL alcohol; pH range light brown-yellow 3.8–6.6 rose.

**Glyoxylic acid solution** (protein detection): cover 10 g of magnesium powder with water and slowly add 250 mL of a saturated oxalic solution, keeping the mixture cool; filter off the magnesium oxalate, acidify the filtrate with acetic acid and make up to a liter with water.

**Guaiacum tincture**: dissolve 1 g of guaiacum in 100 mL of alcohol.

**Gunzberg's reagent** (detection of HCl in gastric juice): dissolve 4 g of phloroglucinol and 2 g of vanillin in 100 mL of absolute alcohol; use only a freshly prepared solution.

**Hager's reagent** (for alkaloids): this reagent is a saturated solution of picric acid in water.

**Hanus solution** (for determination of iodine number): dissolve 13.2 g of iodine in a liter of glacial acetic acid that will not reduce chromic acid; add sufficient bromine to double the halogen content determined by titration (3 mL is about the right amount). The iodine may be dissolved with the aid of heat, but the solution must be cold when the bromine is added.

**Hematoxylin** (indicator): dissolve 0.5 g in 100 mL alcohol; pH range yellow 5.0–6.0.

**Heptamethoxy red**, 2,4,6,2',4',2'',4''-heptamethoxytriphenyl carbinol (indicator): dissolve 0.1 g in 100 mL alcohol; pH range red 5.0–7.0 colorless.

**Hydriodic acid**, HI—0.5*N*: 64 g per liter.

**Hydrobromic acid**, HBr—0.5*N*: 40 g per liter.

**Hydrochloric acid**, HCl—5*N*: 182 g per liter; sp. gr. 1.084.

**Hydrofluoric acid**,  $\text{H}_2\text{F}_2$ —48% solution: use as purchased, and keep in the special container.

**Hydrogen peroxide**,  $\text{H}_2\text{O}_2$ —3% solution: use as purchased.

**Hydrogen sulfide**,  $\text{H}_2\text{S}$ : prepare a saturated aqueous solution.

**Indicator solutions:** a number of indicator solutions are listed in this section under the names of the indicators; e.g., alizarin, aurin, azolitmin, et al., which follow alphabetically. *See also* various index entries.

**Indigo carmine**, sodium indigodisulfonate (indicator): dissolve 0.25 g in 100 mL 50% alcohol; pH range blue 11.6–14.0 yellow.

**Indo-oxine**, 5,8-quinolinequinone-8-hydroxy-5-quinoyl-5-imide (indicator): dissolve 0.05 g in 100 mL alcohol; pH range red 6.0–8.0 blue. Cf. Berg and Becker, *Z. Anal. Chem.* **119**:81 (1940).

**Iodeosin**, tetraiodofluorescein (indicator): dissolve 0.1 g in 100 mL ether saturated with water; pH range yellow 0—about 4 rose-red; *see also* under methyl orange.

**Iodic acid**,  $\text{HIO}_3$ —0.5N ( $\text{HIO}_3/12$ ): 15 g per liter.

**Iodine:** *see* tincture of iodine.

**Lacmoid** (indicator): dissolve 0.5 g in 100 mL alcohol; pH range red 4.4–6.2 blue.

**Lead acetate**,  $\text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$ —0.5N: 95 g per liter.

**Lead chloride**,  $\text{PbCl}_2$ —saturated solution is 1/7N.

**Lead nitrate**,  $\text{Pb}(\text{NO}_3)_2$ —0.5N: 83 g per liter.

**Lime water:** *see* calcium hydroxide.

**Litmus** (indicator): powder the litmus and make up a 2% solution in water by boiling for 5 minutes; pH range red 4.5–8.3 blue.

**Magnesia mixture:** 100 g of  $\text{MgSO}_4$ , 200 g of  $\text{NH}_4\text{Cl}$ , 400 mL of  $\text{NH}_4\text{Cl}$ , 800 mL of water; each mL  $\equiv$  0.01 g phosphorus (P).

**Magnesium chloride**,  $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 50 g per liter.

**Magnesium nitrate**,  $\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 64 g per liter.

**Magnesium sulfate**, epsom salts,  $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ —0.5N: 62 g per liter; saturated solution dissolve 600 g of the salt in water and dilute to 1 liter.

**Manganous chloride**,  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ —0.5N: 50 g per liter.

**Manganous nitrate**,  $\text{Mn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 72 g per liter.

**Manganous sulfate**,  $\text{MnSO}_4 \cdot 7\text{H}_2\text{O}$ —0.5N: 69 g per liter.

**Marme's reagent** (gives yellowish-white precipitate with salts of alkaloids): saturate a boiling solution of 4 parts of KI in 12 parts of water with  $\text{CdI}_2$ ; then add an equal volume of cold saturated KI solution.

**Marquis reagent** (gives a purple-red coloration, then violet, then blue with morphine, codeine, dionine, and heroine): mix 3 mL of concentrated  $\text{H}_2\text{SO}_4$  with 3 drops of a 35% formaldehyde solution.

**Mayer's reagent** (gives white precipitate with most alkaloids in a slightly acid solution): dissolve 13.55 g of  $\text{HgCl}_2$  and 50 g of KI in a liter of water.

**Mercuric chloride**,  $\text{HgCl}_2$ —0.5N: 68 g per liter.

**Mercuric nitrate**,  $\text{Hg}(\text{NO}_3)_2$ —0.5N: 81 g per liter.

**Mercuric sulfate**,  $\text{HgSO}_4$ —0.5N: 74 g per liter.

**Mercurous nitrate**,  $\text{HgNO}_3$ : mix 1 part of  $\text{HgNO}_3$ , 20 parts of  $\text{H}_2\text{O}$ , and 1 part of  $\text{HNO}_3$ .

**Metacresol purple**, *m*-cresol-sulfonphthalein (indicator): dissolve 0.1 g in 13.6 mL 0.02N NaOH and dilute with water to 250 mL; acid pH range red 0.5–2.5 yellow, alkaline pH range yellow 7.4–9.0 purple.

**Metanil yellow**, diphenylaminoazo-*m*-benzene sulfonic acid (indicator): dissolve 0.25 g in 100 mL alcohol; pH range red 1.2–2.3 yellow.

**Methyl green**, hexamethylpararosanine hydroxymethylate (component of mixed indicator): dissolve 0.1 g in 100 mL alcohol; when used with equal parts of hexamethoxytriphenyl carbinol gives color change from violet to green at a titration exponent (pI) of 4.0.

**Methyl orange**, orange III, tropeolin D, sodium *p*-dimethylaminoazobenzenesulfonate (indicator): dissolve 0.1 g in 100 mL water; pH range red 3.0–4.4 orange-yellow. If during a titration where methyl yellow is being used a precipitate forms which tends to remove the indicator from the aqueous phase, methyl orange will be found to be a more suitable indicator. This occurs, for example, in titrations of soaps with acids. The fatty acids, liberated by the titration, extract the methyl yellow so that the endpoint cannot be perceived. Likewise methyl orange is more suitable for titrations in the presence of immiscible organic solvents such as carbon tetrachloride or ether used in the extraction of alkaloids for analysis. Iodeosin (*q.v.*) has also been proposed as an indicator for such cases. Cf. Mylius and Foerster, *Ber.* **24**:1482 (1891); *Z. Anal. Chem.* **31**:240 (1892).

**Methyl red**, *p*-dimethylaminoazobenzene-*o*'-carboxylic acid (indicator): dissolve 0.1 g in 18.6 mL of 0.02N NaOH and dilute with water to 250 mL; or, 0.1 g in 60% alcohol; pH range red 4.4–6.2 yellow.

**Methyl violet** (indicator): dissolve 0.25 g in 100 mL water, pH range blue 1.5–3.2 violet.

**Methyl yellow**, *p*-dimethylaminoazobenzene, benzeneazodimethylaniline (indicator): dissolve 0.1 g in 200 mL alcohol; pH range red 2.9–4.0 yellow. The color change from yellow to orange can be perceived somewhat more sharply than the change of methyl orange from orange to rose, so that methyl yellow seems to deserve preference in many cases. *See also* under methyl orange.

**Methylene blue**, *N,N,N',N'*-tetramethylthionine (component of mixed indicator): dissolve 0.1 g in 100 mL alcohol; when used with equal part of methyl yellow gives color change from blue-violet to green at a titration exponent (pI) of 3.25; when used with equal part of 0.2% methyl red in alcohol gives color change from red-violet to green at a titration exponent (pI) of 5.4; when used with an equal part of neutral red gives color change from violet-blue to green at a titration exponent (pI) of 7.0.

**Millon's reagent** (gives a red precipitate with certain proteins and with various phenols): dissolve 1 part of mercury in 1 part of  $\text{HNO}_3$  (sp. gr. 1.40) with gentle heating, then add 2 parts of water; a few crystals of  $\text{KNO}_3$  help to maintain the strength of the reagent.

**Mohr's salt**: *see* ferrous ammonium sulfate.

**$\alpha$ -Naphthol solution**: dissolve 144 g of  $\alpha$ -naphthol in enough alcohol to make a liter of solution.

**$\alpha$ -Naphtholbenzein** (indicator): dissolve 0.1 g in 100 mL 70% alcohol; pH range colorless 9.0–11.0 blue.

**$\alpha$ -Naphtholphthalein** (indicator): dissolve 0.1 g in 50 mL alcohol and dilute with water to 100 mL; pH range pale yellow-red 7.3–8.7 green.

**Nessler's reagent** (for free ammonia): dissolve 50 g of KI in the least possible amount of cold water; add a saturated solution of  $\text{HgCl}_2$  until a very slight excess is indicated; add 400 mL of a 50% solution of KOH; allow to settle, make up to a liter with water, and decant.

**Neutral red**, toluylene red, dimethyldiaminophenazine chloride, aminodimethylaminotoluphenazine hydrochloride (indicator): dissolve 0.1 g in 60 mL alcohol and dilute with water to 100 mL; pH range red 6.8–8.0 yellow-orange.

**Nickel chloride**,  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 59 g per liter.

**Nickel nitrate**,  $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 73 g per liter.

**Nickel sulfate**,  $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ —0.5N: 66 g per liter.

**Nitramine**, picrylmethylnitramine, 2,4,6-trinitrophenylmethyl nitramine (indicator): dissolve 0.1 g in 60 mL alcohol and dilute with water to 100 mL; pH range colorless 10.8–13.0 red-brown; the solution should be kept in the dark as nitramine is unstable; on boiling with alkali it decomposes quickly. Fresh solutions should be prepared every few months.

**Nitric acid**,  $\text{HNO}_3$ —5N: 315 g per liter; sp. gr. 1.165.

**Nitrohydrochloric acid**: see aqua regia.

**p-Nitrophenol** (indicator): dissolve 0.2 g in 100 mL water; pH range colorless at about 5–7 yellow.

**Nitroso- $\beta$ -naphthol**,  $\text{HOC}_{10}\text{H}_6\text{NO}$ —saturated solution: saturate 100 mL of 50% acetic acid with the solid.

**Nylander's solution** (detection of glucose): dissolve 40 g of rochelle salt and 20 g of bismuth subnitrate in 1000 mL of an 8% NaOH solution.

**Obermayer's reagent** (detection of indoxyl in urine): dissolve 4 g of  $\text{FeCl}_3$  in a liter of concentrated HCl.

**Orange III** (indicator): see under methyl orange.

**Oxalic acid**,  $\text{H}_2\text{C}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ : dissolve in ten parts of water.

**Pavy's solution** (estimation of glucose): mix 120 mL of Fehling's solution and 300 mL of ammonium hydroxide (sp. gr. 0.88), and dilute to a liter with water.

**Perchloric acid**,  $\text{HClO}_4$ —60%: use as purchased.

**Phenol red**, phenol-sulfonphthalein (indicator): dissolve 0.1 g in 14.20 mL 0.02N NaOH and dilute with water to 250 mL; or, 0.1 g in 100 mL 20% alcohol; pH range yellow 6.8–8.0 red.

**Phenol solution**: dissolve 20 g of phenol (carbolic acid) in a liter of water.

**Phenol sulfonic acid** (determination of nitrogen as nitrate; water analysis for nitrate): dissolve 25 g pure, white phenol in 150 mL of pure concentrated  $\text{H}_2\text{SO}_4$ , add 75 mL of fuming  $\text{H}_2\text{SO}_4$  (15%  $\text{SO}_3$ ), stir well and heat for two hours at 100°C.

**Phenolphthalein** (indicator): dissolve 1 g in 60 mL of alcohol and dilute with water to 100 mL; pH range colorless 8.2–10.0 red.

**Phosphoric acid**, *ortho*,  $\text{H}_3\text{PO}_4$ —0.5N: 16 g per liter.

**Poirrer blue C4B** (indicator): dissolve 0.2 g in 100 mL water; pH range blue 11.0–13.0 red.

**Potassium acid antimonate**,  $\text{KH}_2\text{SbO}_4$ —0.1N: boil 23 g of the salt with 950 mL of water for 5 minutes, cool rapidly and add 35 mL of 6N KOH; allow to stand for one day, filter dilute filtrate to a liter.

**Potassium arsenate**,  $\text{K}_3\text{AsO}_4$ —0.5N ( $\text{K}_3\text{AsO}_4/10$ ): 26 g per liter.

**Potassium arsenite**,  $\text{KAsO}_2$ —0.5N ( $\text{KAsO}_2/6$ ): 24 g per liter.

**Potassium bromate**,  $\text{KBrO}_3$ —0.5N ( $\text{KBrO}_3/12$ ): 14 g per liter.

**Potassium bromide**,  $\text{KBr}$ —0.5N: 60 g per liter.



**Potassium carbonate**,  $\text{K}_2\text{CO}_3$ —3*N*: 207 g per liter.

**Potassium chloride**,  $\text{KCl}$ —0.5*N*: 37 g per liter.

**Potassium chromate**,  $\text{K}_2\text{CrO}_4$ —0.5*N*: 49 g per liter.

**Potassium cyanide**,  $\text{KCN}$ —0.5*N*: 33 g per liter.

**Potassium dichromate**,  $\text{K}_2\text{Cr}_2\text{O}_7$ —0.5*N* ( $\text{K}_2\text{Cr}_2\text{O}_7/8$ ): 38 g per liter.

**Potassium ferricyanide**,  $\text{K}_3\text{Fe}(\text{CN})_6$ —0.5*N*: 55 g per liter.

**Potassium ferrocyanide**,  $\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$ —0.5*N*: 53 g per liter.

**Potassium hydroxide**,  $\text{KOH}$ —5*N*: 312 g per liter.

**Potassium iodate**,  $\text{KIO}_3$ —0.5*N* ( $\text{KIO}_3/12$ ): 18 g per liter.

**Potassium iodide**,  $\text{KI}$ —0.5*N*: 83 g per liter.

**Potassium nitrate**,  $\text{KNO}_3$ —0.5*N*: 50 g per liter.

**Potassium nitrate**,  $\text{KNO}_2$ —6*N*: 510 g per liter.

**Potassium permanganate**,  $\text{KMnO}_4$ —0.5*N* ( $\text{KMnO}_4/10$ ): 16 g per liter.

**Potassium pyrogallate** (oxygen in gas analysis): weigh out 5 g of pyrogallol (pyrogallic acid), and pour upon it 100 mL of a  $\text{KOH}$  solution. If the gas contains less than 28% of oxygen, the  $\text{KOH}$  solution should be 500 g  $\text{KOH}$  in a liter of water; if there is more than 28% of oxygen in the gas, the  $\text{KOH}$  solution should be 120 g of  $\text{KOH}$  in 100 mL of water.

**Potassium sulfate**,  $\text{K}_2\text{SO}_4$ —0.5*N*: 44 g per liter.

**Potassium thiocyanate**,  $\text{KCNS}$ —0.5*N*: 49 g per liter.

**Precipitating reagent** (for group II, anions): dissolve 61 g of  $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$  and 52 g of  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  in water and dilute to 1 liter. If the solution becomes turbid, filter and use filtrate.

**Quinaldine red** (indicator): dissolve 0.1 g in 100 mL alcohol; pH range colorless 1.4–3.2 red.

**Quinoline blue**, cyanin (indicator): dissolve 1 g in 100 mL alcohol; pH range colorless 6.6–8.6 blue.

**Rosolic acid**, aurin, corallin, corallinphthalein, 4,4'-dihydroxy-fuchsone, 4,4'-dihydroxy-3-methyl-fuchsone (indicator): dissolve 0.5 g in 50 mL alcohol and dilute with water to 100 mL.

**Salicyl yellow** (indicator): *see* alizarin yellow GG.

**Scheibler's reagent** (precipitates alkaloids, albumoses and peptones): dissolve sodium tungstate in boiling water containing half its weight of phosphoric acid (sp. gr. 1.13); on evaporation of this solution, crystals of phosphotungstic acid are obtained. A 10% solution of phosphotungstic acid in water constitutes the reagent.

**Schweitzer's reagent** (dissolves cotton, linen, and silk, but not wool); add  $\text{NH}_4\text{Cl}$  and  $\text{NaOH}$  to a solution of copper sulfate. The blue precipitate is filtered off, washed, pressed, and dissolved in ammonia (sp. gr. 0.92).

**Silver nitrate**,  $\text{AgNO}_3$ —0.25*N*: 43 g per liter.

**Silver sulfate**,  $\text{Ag}_2\text{SO}_4$ —*N*/13 (saturated solution): stir mechanically 10 g of the salt in a liter of water for 3 hours; decant and use the clear liquid.

**Soap solution** (for hardness in water): (*a*) *Clark's or A.P.H.A. Stand. Methods*—prepare stock solution of 100 g of pure powdered castile soap in a liter of 80% ethyl alcohol; allow to stand over night and decant. Titrate against  $\text{CaCl}_2$  solution (0.5 g  $\text{CaCO}_3$  dissolved in a concentrated  $\text{HCl}$ , neutralized with  $\text{NH}_4\text{OH}$  to slight alkalinity using litmus as the indicator, make up to 500 mL; 1 mL of this solution is equivalent to 1 mg  $\text{CaCO}_3$ ) and dilute with 80% alcohol until 1 mL of the resulting solution is equivalent to 1 mL of the standard  $\text{CaCl}_2$  making due allowance

for the lather factor (the lather factor is that amount of standard soap solution required to produce a permanent lather in a 50-mL portion of distilled water). One milliliter of this solution after subtracting the lather factor is equivalent to 1 mg of  $\text{CaCO}_3$ . (b) *Boutron-Boudet*—dissolve 100 g of pure castile soap in about 2500 mL of 56% ethyl alcohol and adjust so that 2.4 mL will give a permanent lather with 40 mL of a solution containing 0.59 g  $\text{Ba}(\text{NO}_3)_2$  per liter of water; 2.4 mL of this solution is equivalent to 22 French degrees or 220 parts per million of hardness (as  $\text{CaCO}_3$ ) on a 40-mL sample of water.

**Sodium acetate**,  $\text{NaC}_2\text{H}_3\text{O}_2 \cdot 3\text{H}_2\text{O}$ : dissolve 1 part of the salt in 10 parts of water.

**Sodium acetate, acid**: dissolve 100 g of sodium acetate and 30 mL of glacial acetic acid in water and dilute to 1 liter.

**Sodium bismuthate** (oxidation of manganese): heat 20 parts of  $\text{NaOH}$  nearly to redness in an iron or nickel crucible, and add slowly 10 parts of basic bismuth nitrate which has been previously dried. Add 2 parts of sodium peroxide, and pour the brownish-yellow fused mass on an iron plate to cool. When cold break up in a mortar, extract with water, and collect on an asbestos filter.

**Sodium carbonate**,  $\text{Na}_2\text{CO}_3 \cdot 3\text{H}_2\text{O}$ : 159 g per liter; one part  $\text{Na}_2\text{CO}_3$ , or 2.7 parts of the crystalline  $\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$  in 5 parts of water.

**Sodium chloride**,  $\text{NaCl}$ —0.5N: 29 g per liter.

**Sodium chloroplatinite**,  $\text{Na}_2\text{PtCl}_4$ : dissolve 1 part of the salt in 12 parts of water.

**Sodium cobaltinitrite**,  $\text{Na}_2\text{Co}(\text{NO}_2)_6$ —0.3N: dissolve 230 g of  $\text{NaNO}_2$  in 500 mL of water, add 160 mL of 6N acetic acid and 35 g of  $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ . Allow to stand one day, filter, and dilute the filtrate to a liter.

**Sodium hydrogen phosphate**,  $\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$ —0.5N: 60 g liter.

**Sodium hydroxide**,  $\text{NaOH}$ —5N: 220 g per liter.

**Sodium hydroxide, alcoholic**: dissolve 20 g of  $\text{NaOH}$  in alcohol and dilute to 1 liter with alcohol.

**Sodium hypobromite**: dissolve 100 g of  $\text{NaOH}$  in 250 mL of water and add 25 mL of bromine.

**Sodium nitrate**,  $\text{NaNO}_3$ —0.5N: 43 g per liter.

**Sodium nitroprusside** (for sulfur detection): dissolve about 1 g of sodium nitroprusside in 10 mL of water; as the solution deteriorates on standing, only freshly prepared solutions should be used. This compound is also called sodium nitroferrocyanide and has the formula  $\text{Na}_2\text{Fe}(\text{NO})(\text{CN})_5 \cdot 2\text{H}_2\text{O}$ .

**Sodium polysulfide**,  $\text{Na}_2\text{S}_x$ : dissolve 480 g of  $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$  in 500 mL of water, add 40 g of  $\text{NaOH}$  and 18 g of sulfur, stir mechanically and dilute to 1 liter with water.

**Sodium sulfate**,  $\text{Na}_2\text{SO}_4$ —0.5N: 35 g per liter.

**Sodium sulfide**,  $\text{Na}_2\text{S}$ : saturate  $\text{NaOH}$  solution with  $\text{H}_2\text{S}$ , then add as much  $\text{NaOH}$  as was used in the original solution.

**Sodium sulfite**,  $\text{Na}_2\text{SO}_3 \cdot 7\text{H}_2\text{O}$ —0.5N: 63 g per liter.

**Sodium sulfite, acid** (saturated): dissolve 600 g of  $\text{NaHSO}_3$  in water and dilute to 1 liter; for the preparation of addition compounds with aldehydes and ketones: prepare a saturated solution of sodium carbonate in water and saturate with sulfur dioxide.

**Sodium tartrate, acid**,  $\text{NaHC}_4\text{H}_4\text{O}_6$ : dissolve 1 part of the salt in 10 parts of water.

**Sodium thiosulfate**,  $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ : one part of the salt in 40 parts of water.

**Sonnenschein's reagent** (alkaloid detection): a nitric acid solution of ammonium molybdate is treated with phosphoric acid. The precipitate so produced is washed and boiled with aqua regia

until the ammonium salt is decomposed. The solution is evaporated to dryness and the residue is dissolved in 10%  $\text{HNO}_3$ .

**Stannic chloride**,  $\text{SnCl}_4$ —0.5N: 33 g per liter.

**Stannous chloride**,  $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ —0.5N: 56 g per liter. The water should be acid with  $\text{HCl}$  and some metallic tin should be kept in the bottle.

**Starch solution** (iodine indicator): dissolve 5 g of soluble starch in cold water, pour the solution into 2 liters of water and boil for a few minutes. Keep in a glass-stoppered bottle.

**Starch solution** (other than soluble): make a thin paste of the starch with cold water, then stir in 200 times its weight of boiling water and boil for a few minutes. A few drops of chloroform added to the solution acts as a preservative.

**Stoke's reagent**: dissolve 30 g of ferrous sulfate and 20 g of tartaric acid in water and dilute to 1 liter. When required for use, add strong ammonia until the precipitate first formed is dissolved.

**Strontium chloride**,  $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 67 g per liter.

**Strontium nitrate**,  $\text{Sr}(\text{NO}_3)_2$ —0.5N: 53 g per liter.

**Strontium sulfate**,  $\text{SrSO}_4$ : prepare a saturated solution.

**Sulfanilic acid** (for detection of nitrites): dissolve 8 g of sulfanilic acid in 1 liter of acetic acid (sp. gr. 1.04).

**Sulfuric acid**,  $\text{H}_2\text{SO}_4$ —5N: 245 g per liter, sp. gr. 1.153.

**Sulfurous acid**,  $\text{H}_2\text{SO}_3$ : saturate water with sulfur dioxide.

**Tannic acid**: dissolve 1 g tannic acid in 1 mL alcohol and make up to 10 mL with water.

**Tartaric acid**,  $\text{H}_2\text{C}_4\text{H}_4\text{O}_6$ : dissolve one part of the acid in 3 parts of water; for a saturated solution dissolve 750 g of tartaric acid in water and dilute to 1 liter.

**Tetrabromophenol blue**, tetrabromophenol-tetrabromosulfonphthalein (indicator): dissolve 0.1 g in 5 mL 0.02N  $\text{NaOH}$  and dilute with water to 250 mL; pH range yellow 3.0–4.6 blue.

**Thymol blue**, thymol-sulfonphthalein (indicator): dissolve 0.1 g in 10.75 mL 0.02N  $\text{NaOH}$  and dilute with water to 250 mL; or dissolve 0.1 g in 20 mL warm alcohol and dilute with water to 100 mL; pH range (acid) red 1.2–2.8 yellow, and (alkaline) yellow 8.0–9.6 blue.

**Thymolphthalein** (indicator): dissolve 0.1 g in 100 mL alcohol; pH range colorless 9.3–10.5 blue.

**Tincture of iodine** (antiseptic): add 70 g of iodine and 50 g of  $\text{KI}$  to 50 mL of water; make up to 1 liter with alcohol.

**o-Tolidine solution** (for residual chlorine in water analysis): dissolve 1 g of pulverized o-tolidine, m.p.  $129^\circ\text{C}$ ., in 1 liter of dilute hydrochloric acid (100 mL conc.  $\text{HCl}$  diluted to 1 liter).

**Toluylene red** (indicator): see neutral red.

**Trichloroacetic acid**: dissolve 100 g of the acid in water and dilute to 1 liter.

**Trinitrobenzene**, 1,3,5-trinitrobenzene (indicator): dissolve 0.1 g in 100 mL alcohol; pH range colorless 11.5–14.0 orange.

**Trinitrobenzoic acid**, 2,4,6-trinitrobenzoic acid (indicator): dissolve 0.1 g in 100 mL water; pH range colorless 12.0–13.4 orange-red.

**Tropeolin D** (indicator): see methyl orange.

**Tropeolin O**, sodium 2,4-dihydroxyazobenzene-4-sulfonate (indicator): dissolve 0.1 g in 100 mL water; pH range yellow 11.0–13.0 orange-brown.

**Tropeolin OO**, orange IV, sodium *p*-diphenylamino-azobenzene sulfonate, sodium 4'-anilino-azobenzene-4-sulfonate (indicator): dissolve 0.1 g in 100 mL water; pH range red 1.3–3.2 yellow.

**Tropeolin OOO**, sodium  $\alpha$ -naphtholazobenzene sulfonate (indicator): dissolve 0.1 g in 100 mL water; pH range yellow 7.6–8.9 red.

**Turmeric paper** (gives a rose-brown coloration with boric acid): wash the ground root of turmeric with water and discard the washings. Digest with alcohol and filter, using the clear filtrate to impregnate white, unsized paper, which is then dried.

**Uffelmann's reagent** (gives a yellow coloration in the presence of lactic acid): add a ferric chloride solution to a 2% phenol solution until the solution becomes violet in color.

**Wagner's solution** (phosphate rock analysis): dissolve 25 g citric acid and 1 g salicylic acid in water, and make up to 1 liter. Twenty-five to fifty milliliters of this reagent prevents precipitation of iron and aluminum.

**Wijs solution** (for iodine number): dissolve 13 g resublimed iodine in 1 liter of glacial acetic acid (99.5%), and pass in washed and dried (over or through  $\text{H}_2\text{SO}_4$ ) chlorine gas until the original thio titration of the solution is not quite doubled. There should be only a slight excess of iodine and no excess of chlorine. Preserve the solution in amber colored bottles sealed with paraffin. Do not use the solution after it has been prepared for more than 30 days.

**Xylene cyanole-methyl orange indicator**, Schoepfle modification (for partially color blind operators): dissolve 0.75 g xylene cyanole FF (Eastman No. T 1579) and 1.50 g methyl orange in 1 liter of water.

***p*-Xylenol blue**, 1,4-dimethyl-5-hydroxybenzene-sulfonphthalein (indicator): dissolve 0.1 g in 250 mL alcohol; pH range (acid) red 1.2–2.8 yellow, and (alkaline) yellow 8.0–9.6 blue.

**Zinc chloride**,  $\text{ZnCl}_2$ —0.5N: 34 g per liter.

**Zinc nitrate**,  $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ —0.5N: 74 g per liter.

**Zinc sulfate**,  $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ —0.5N: 72 g per liter.

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors

Exposure limits (threshold limit value or TLV) are those set by the Occupational Safety and Health Administration and represent conditions to which most workers can be exposed without adverse effects. The TLV value is expressed as a time weighted average airborne concentration over a normal 8-hour workday and 40-hour work-week.

| Substance        | Maximum allowable exposure |                                 | Toxicity          |
|------------------|----------------------------|---------------------------------|-------------------|
|                  | ppm                        | $\text{mg} \cdot \text{m}^{-3}$ |                   |
| Acetaldehyde     | 25                         | 45                              | carcinogen        |
| Acetic acid      | 10                         | 25                              |                   |
| Acetic anhydride | 5                          | 21                              |                   |
| Acetone          | 750                        | 1780                            |                   |
| Acetonitrile     | 40                         | 67                              |                   |
| Acetophenone     | 10                         | 49                              | slightly narcotic |
| Acetylene        |                            |                                 |                   |
| Acrolein         | 0.1                        | 0.23                            |                   |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                                          | Maximum allowable exposure |                      | Toxicity                           |
|----------------------------------------------------|----------------------------|----------------------|------------------------------------|
|                                                    | ppm                        | mg · m <sup>-3</sup> |                                    |
| Acrylic acid                                       | 2                          | 5.9                  |                                    |
| Acrylonitrile                                      | 2                          | 4.3                  |                                    |
| Acrylonitrile                                      | 20                         | 45                   |                                    |
| Allyl alcohol                                      | 2                          | 4.8                  |                                    |
| Allyl chloride                                     | 1                          | 3                    |                                    |
| Allyl glycidyl ether                               | 5                          | 22                   |                                    |
| Ammonia                                            | 25                         | 18                   | toxic                              |
| Aniline                                            | 2                          | 7.6                  | carcinogen                         |
| Arsine                                             | 0.05                       | 0.2                  | highly toxic                       |
| Benzene                                            | 10                         | 32                   | carcinogen                         |
| Benzenethiol                                       | 0.5                        | 2.3                  |                                    |
| <i>p</i> -Benzoquinone                             | 0.1                        |                      |                                    |
| Benzoyl chloride                                   | 0.5                        |                      |                                    |
| Benzoyl peroxide                                   |                            | 5                    |                                    |
| Benzyl acetate                                     | 10                         |                      |                                    |
| Benzyl chloride                                    | 1                          |                      | carcinogen                         |
| Biphenyl                                           | 0.2                        |                      |                                    |
| Bis(2-aminoethyl)amine                             | 1                          |                      |                                    |
| Bis(2-chloroethyl) ether                           | 5                          | 29                   |                                    |
| Bis(2-chloromethyl) ether                          | 0.001                      |                      | carcinogen                         |
| Bis(2-ethylhexyl) phthalate                        |                            | 5                    |                                    |
| Boron tribromide                                   | 1                          |                      |                                    |
| Boron trichloride                                  |                            |                      | toxic                              |
| Boron trifluoride                                  | 1                          | 3                    | highly toxic                       |
| Bromine                                            | 0.1                        | 0.7                  |                                    |
| Bromine pentafluoride                              | 0.1                        |                      | highly toxic                       |
| Bromine trifluoride                                |                            |                      | highly toxic                       |
| Bromochloromethane (Halon 1011)                    | 200                        | 1060                 |                                    |
| Bromoethane                                        | 5                          | 22                   | carcinogen                         |
| Bromoethylene                                      | 5                          | 22                   | slightly toxic                     |
| Bromoform                                          | 0.5                        | 5                    |                                    |
| Bromomethane                                       | 5                          | 19                   | highly toxic,<br>carcinogen        |
| 1,3-Butadiene                                      | 2                          |                      | slightly anesthetic,<br>carcinogen |
| Butane                                             | 800                        | 1900                 | slightly anesthetic                |
| 1-Butanethiol                                      | 0.5                        | 1.8                  |                                    |
| 1-Butanol                                          | 50                         | 152                  |                                    |
| 2-Butanol                                          | 100                        | 303                  |                                    |
| 2-Butanone                                         | 200                        | 590                  |                                    |
| 2-Butoxyethanol                                    | 25                         | 121                  |                                    |
| Butyl acetate                                      | 150                        | 710                  |                                    |
| <i>sec</i> -Butyl acetate                          | 200                        | 950                  |                                    |
| <i>tert</i> -Butyl acetate                         | 200                        | 950                  |                                    |
| Butyl acrylate                                     | 10                         |                      |                                    |
| <i>tert</i> -Butyl alcohol                         | 100                        | 300                  |                                    |
| Butylamine                                         | 5                          | 15                   |                                    |
| <i>tert</i> -Butyl chromate (as CrO <sub>3</sub> ) |                            | 0.1                  |                                    |
| Butyl glycidyl ether                               | 50                         | 270                  |                                    |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                                            | Maximum allowable exposure |                      | Toxicity          |
|------------------------------------------------------|----------------------------|----------------------|-------------------|
|                                                      | ppm                        | mg · m <sup>-3</sup> |                   |
| Butyl mercaptan                                      | 0.5                        | 1.5                  |                   |
| <i>p</i> -tert-Butyltoluene                          | 10                         |                      |                   |
| (+)-Camphor                                          | 2                          | 12                   |                   |
| Caprolactam                                          | 5                          |                      |                   |
| Carbon dioxide                                       | 5000                       | 9000                 |                   |
| Carbon disulfide                                     | 10                         | 31                   |                   |
| Carbon monoxide                                      | 25                         | 28                   | toxic             |
| Carbon tetrachloride                                 | 10                         | 65                   |                   |
| Carbonyl chloride                                    | 0.1                        |                      |                   |
| Carbonyl fluoride                                    | 2                          |                      | toxic             |
| Chlordane                                            |                            | 0.5                  |                   |
| Chlorine                                             | 0.5                        | 1.5                  | highly toxic      |
| Chlorine dioxide                                     | 0.1                        | 0.3                  |                   |
| Chlorine trifluoride                                 | 0.1                        | 0.4                  | highly toxic      |
| Chloroacetaldehyde                                   | 1                          | 3                    |                   |
| $\alpha$ -Chloroacetophenone                         | 0.05                       | 0.3                  |                   |
| Chloroacetyl chloride                                | 0.05                       |                      |                   |
| Chlorobenzene                                        | 10                         | 46                   |                   |
| 2-Chloro-1,3-butadiene                               | 10                         |                      | carcinogen        |
| Chlorodifluoromethane (CFC 22)                       | 1000                       | 3540                 |                   |
| Chloroethane                                         | 100                        | 264                  | low toxicity      |
| 2-Chloroethanol                                      | 1                          | 3.3                  |                   |
| Chloroethylene (vinyl chloride)                      | 5                          | 13                   | toxic, carcinogen |
| Chloroform (trichloromethane)                        | 10                         | 49                   |                   |
| Chloromethane                                        | 50                         | 103                  | toxic, carcinogen |
| 1-Chloro-1-nitropropane                              | 20                         | 100                  |                   |
| Chloropentafluoroethane (CFC 115)                    | 1000                       | 6320                 |                   |
| 3-Chloro-1-propene (allyl chloride)                  | 1                          | 3                    | carcinogen        |
| <i>o</i> -Chlorotoluene                              | 50                         | 259                  |                   |
| Chlorotrifluoroethylene                              |                            |                      | toxic             |
| Chromyl chloride (CrO <sub>2</sub> Cl <sub>2</sub> ) | 0.025                      |                      | carcinogen        |
| <i>o</i> -Cresol (also <i>m</i> -, <i>p</i> -)       | 5                          | 22                   |                   |
| <i>trans</i> -Crotonaldehyde                         | 2                          | 5.7                  |                   |
| Cyanogen                                             | 10                         | 20                   | highly toxic      |
| Cyanogen chloride                                    | 0.3                        |                      |                   |
| Cyclohexane                                          | 300                        | 1030                 |                   |
| Cyclohexanol                                         | 50                         | 206                  |                   |
| Cyclohexanone                                        | 25                         | 100                  |                   |
| Cyclohexene                                          | 300                        | 1015                 |                   |
| Cyclohexylamine                                      | 10                         | 41                   |                   |
| 1,3-Cyclopentadiene                                  | 75                         |                      |                   |
| Cyclopentane                                         | 600                        | 1720                 |                   |
| Cyclopropane                                         |                            |                      | anesthetic        |
| 2,4-D                                                |                            | 10                   |                   |
| DDT                                                  |                            | 1                    |                   |
| Decaborane                                           | 0.05                       | 0.3                  |                   |
| Diacetone alcohol                                    | 50                         | 238                  |                   |
| 2,2'-Diaminodiethylamine                             | 1                          | 4.2                  |                   |
| Diazomethane                                         | 0.2                        |                      | carcinogen        |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                                       | Maximum allowable exposure |                      | Toxicity                      |
|-------------------------------------------------|----------------------------|----------------------|-------------------------------|
|                                                 | ppm                        | mg · m <sup>-3</sup> |                               |
| Diborane                                        | 0.1                        | 0.1                  |                               |
| Dibromodifluoromethane                          | 100                        | 860                  |                               |
| 1,2-Dibromoethane                               |                            |                      | carcinogen                    |
| Dibutyl phthalate                               |                            | 5                    |                               |
| Dichloroacetylene                               | 0.1                        |                      |                               |
| <i>o</i> -Dichlorobenzene                       | 25                         | 150                  |                               |
| <i>p</i> -Dichlorobenzene                       | 10                         | 60                   | carcinogen                    |
| Dichlorodifluoromethane (Freon 12)              | 1000                       | 4950                 |                               |
| 1,1-Dichloroethane                              | 100                        | 405                  |                               |
| 1,2-Dichloroethane                              | 10                         | 40                   | carcinogen                    |
| 1,1-Dichloroethylene                            | 5                          | 20                   | carcinogen                    |
| <i>cis</i> -1,2-Dichloroethylene                | 200                        | 793                  |                               |
| <i>trans</i> -1,2-Dichloroethylene              | 200                        | 793                  |                               |
| Dichlorofluoromethane (Freon 21)                | 10                         | 42                   |                               |
| Dichloromethane                                 | 50                         | 174                  | carcinogen                    |
| 1,1-Dichloro-1-nitroethane                      | 10                         | 60                   |                               |
| 1,2-Dichloropropane                             | 75                         | 347                  | carcinogen                    |
| 1,3-Dichloropropene                             | 1                          |                      | carcinogen                    |
| Dichlorosilane                                  |                            |                      | highly toxic                  |
| 1,2-Dichlorotetrafluoroethane (Freon 114)       | 1000                       | 7000                 |                               |
| Dieldrin                                        |                            | 0.25                 |                               |
| Diethanolamine                                  | 0.46                       |                      |                               |
| Diethylamine                                    | 5                          | 15                   |                               |
| Diethyl ether                                   | 400                        | 1210                 |                               |
| Diglycidyl ether                                | 0.5                        | 2.8                  |                               |
| Diisobutyl ketone                               | 25                         | 150                  |                               |
| Diisopropylamine                                | 5                          | 20                   |                               |
| Diiopropyl ether                                | 250                        | 1040                 |                               |
| Dimethoxymethane                                | 1000                       | 3110                 |                               |
| <i>N,N</i> -Dimethylacetamide                   | 10                         | 35                   |                               |
| Dimethylamine                                   | 5                          | 9.2                  | highly toxic                  |
| <i>N,N</i> -Dimethylaniline                     | 5                          | 25                   |                               |
| Dimethyl 1,2-dibromo-2,2-dichloroethylphosphate |                            | 3                    |                               |
| Dimethyl ether                                  |                            |                      | slightly toxic,<br>anesthetic |
| 1-(1,1-Dimethylethyl)-4-methylbenzene           | 1                          | 6.1                  |                               |
| <i>N,N</i> -Dimethylformamide                   | 10                         | 30                   |                               |
| 2,6-Dimethyl-4-heptanone                        | 25                         |                      |                               |
| 1,1-Dimethylhydrazine                           | 0.5                        | 1                    | carcinogen                    |
| Dimethyl phthalate                              |                            | 5                    |                               |
| 2,2-Dimethylpropane                             |                            |                      | probably anesthetic           |
| Dimethyl sulfate                                | 0.1                        | 0.5                  | carcinogen                    |
| Dinitrobenzene                                  | 0.15                       | 1                    |                               |
| Dinitro- <i>o</i> -cresol                       |                            | 0.2                  |                               |
| Dinitrotoluene                                  |                            | 1.5                  |                               |
| 1,4-Dioxane                                     | 25                         | 90                   | carcinogen                    |
| Diphenyl                                        | 0.2                        | 1                    |                               |
| Diphenyl ether                                  | 1                          | 7                    |                               |
| Dipropylene glycol methyl ether—skin            | 100                        | 600                  |                               |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                         | Maximum allowable exposure |                      | Toxicity          |
|-----------------------------------|----------------------------|----------------------|-------------------|
|                                   | ppm                        | mg · m <sup>-3</sup> |                   |
| Endrin—skin                       |                            | 0.1                  |                   |
| Epichlorohydrin                   | 2                          | 7.6                  | carcinogen        |
| 2,3-Epoxy-1-propanol (glycidol)   | 50                         | 150                  |                   |
| 1,2-Ethanediamine                 | 10                         | 25                   |                   |
| Ethanethiol                       | 0.5                        |                      |                   |
| Ethanol                           | 1000                       | 1880                 |                   |
| Ethanolamine                      | 3                          | 7.5                  |                   |
| 2-Ethoxyethanol (Cellosolve)      | 5                          | 18                   |                   |
| 2-Ethoxyethyl acetate             | 5                          | 27                   |                   |
| Ethyl acetate                     | 400                        | 1400                 |                   |
| Ethyl acrylate                    | 5                          | 20                   |                   |
| Ethylamine                        | 5                          | 9.2                  | highly toxic      |
| Ethylbenzene                      | 100                        | 435                  |                   |
| Ethylene                          |                            |                      | anesthetic        |
| Ethylene glycol                   | 39                         |                      |                   |
| Ethylene glycol dinitrate         | 0.2                        |                      |                   |
| Ethyleneimine                     | 0.05                       |                      | carcinogen        |
| Ethylene oxide                    | 1                          |                      | toxic, carcinogen |
| Ethyl formate                     | 100                        | 300                  |                   |
| Ethyl mercaptan                   | 0.1                        | 1                    |                   |
| Ethyl silicate                    | 100                        | 850                  |                   |
| Fluorine                          | 1                          | 2                    | highly toxic      |
| Fluorotrichloromethane (Freon 11) | 1000                       | 5600                 |                   |
| Formaldehyde                      | 0.3                        |                      | carcinogen        |
| Formamide                         | 10                         | 18                   |                   |
| Formic acid                       | 5                          | 9.4                  |                   |
| 2-Furancarboxaldehyde (furfural)  | 2                          | 7.9                  |                   |
| 2-Furanmethanol                   | 10                         | 40                   |                   |
| Glycerol                          |                            | 10                   |                   |
| Heptachlor                        |                            | 0.5                  |                   |
| Heptane                           | 400                        | 1640                 |                   |
| 2-Heptanone                       | 50                         | 233                  |                   |
| 3-Heptanone                       | 50                         | 234                  |                   |
| Hexachloro-1,3-butadiene          | 0.02                       |                      | carcinogen        |
| Hexachlorocyclohexane (lindane)   |                            | 0.5                  |                   |
| Hexachloroethane                  | 1                          |                      | carcinogen        |
| Hexachloronaphthalene             |                            | 0.2                  |                   |
| Hexamethylphosphoric triamide     |                            |                      | carcinogen        |
| Hexane                            | 50                         | 176                  |                   |
| 2-Hexanone                        | 5                          | 20                   |                   |
| sec-Hexyl acetate                 | 50                         | 300                  |                   |
| Hexylene glycol                   | 25                         |                      |                   |
| Hydrazine                         | 0.01                       | 0.1                  | carcinogen        |
| Hydrogen bromide                  | 3                          | 10                   | highly toxic      |
| Hydrogen chloride                 | 5                          | 7                    | highly toxic      |
| Hydrogen cyanide                  | 4.7                        |                      | highly toxic      |
| Hydrogen fluoride                 | 3                          | 2                    | highly toxic      |
| Hydrogen iodide                   |                            |                      | highly toxic      |
| Hydrogen peroxide (90%)           | 1                          | 1.4                  |                   |



**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                                 | Maximum allowable exposure |                      | Toxicity     |
|-------------------------------------------|----------------------------|----------------------|--------------|
|                                           | ppm                        | mg · m <sup>-3</sup> |              |
| Hydrogen selenide                         | 0.05                       | 0.2                  | highly toxic |
| Hydrogen sulfide                          | 10                         | 15                   | highly toxic |
| 4-Hydroxy-4-methyl-2-pentanone            | 50                         | 238                  |              |
| Indene                                    | 10                         |                      |              |
| Iodine                                    | 0.1                        | 1                    |              |
| Iodine pentafluoride                      |                            |                      | highly toxic |
| Iodomethane                               | 2                          | 12                   |              |
| Isobutyl acetate                          | 150                        | 700                  |              |
| Isobutyl alcohol                          | 50                         | 150                  |              |
| Isopentyl acetate                         | 100                        | 525                  |              |
| Isopentyl alcohol                         | 100                        | 360                  |              |
| Isophorone                                | 5                          | 28                   |              |
| Isopropyl acetate                         | 250                        | 1040                 |              |
| Isopropylamine                            | 5                          | 12                   |              |
| Isopropylbenzene (cumene)                 | 50                         | 246                  |              |
| Isopropyl glycidyl ether                  | 50                         | 240                  |              |
| Ketene                                    | 0.5                        | 0.9                  |              |
| Lindane                                   |                            | 0.5                  |              |
| Liquified petroleum gas                   | 1000                       | 1800                 |              |
| Malathion                                 |                            | 10                   |              |
| Maleic anhydride                          | 0.25                       | 1                    |              |
| Malononitrile                             | 0.05                       | 0.4                  |              |
| Mesityl oxide                             | 15                         | 60                   |              |
| Methacrylic acid                          | 20                         | 70                   |              |
| Methanethiol                              | 0.5                        |                      |              |
| Methanol                                  | 200                        | 262                  |              |
| 2-Methoxyaniline (also 4-)                | 0.1                        |                      | carcinogen   |
| 2-Methoxyethanol                          | 5                          | 16                   |              |
| 2-Methoxyethyl acetate                    | 5                          | 24                   |              |
| Methyl acetate                            | 200                        | 610                  |              |
| Methyl acetylene-propadiene (MAPP)        | 1000                       | 1800                 |              |
| Methyl acrylate                           | 10                         | 35                   |              |
| Methylacrylonitrile                       | 1                          |                      |              |
| Methylamine                               | 5                          | 6.4                  | highly toxic |
| <i>o</i> -Methylaniline (also <i>p</i> -) | 2                          |                      | carcinogen   |
| <i>m</i> -Methylaniline                   | 2                          |                      |              |
| <i>N</i> -Methylaniline                   | 0.5                        | 2.2                  |              |
| 3-Methyl-1-butanol                        | 100                        | 361                  |              |
| Methyl <i>tert</i> -butyl ether           | 40                         |                      |              |
| Methylcyclohexane                         | 400                        | 1600                 |              |
| 1-Methylcyclohexanol                      | 50                         | 234                  |              |
| <i>cis</i> -2-Methylcyclohexanol          | 50                         | 234                  |              |
| <i>trans</i> -2-Methylcyclohexanol        | 50                         | 234                  |              |
| <i>cis</i> -3-Methylcyclohexanol          | 50                         | 234                  |              |
| <i>trans</i> -3-Methylcyclohexanol        | 50                         | 234                  |              |
| <i>cis</i> -4-Methylcyclohexanol          | 50                         | 234                  |              |
| <i>trans</i> -4-Methylcyclohexanol        | 50                         | 234                  |              |
| Methyl formate                            | 100                        | 250                  |              |
| 5-Methyl-2-hexanone                       | 50                         | 234                  |              |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                                             | Maximum allowable exposure |                      | Toxicity     |
|-------------------------------------------------------|----------------------------|----------------------|--------------|
|                                                       | ppm                        | mg · m <sup>-3</sup> |              |
| Methyl hydrazine                                      | 0.01                       |                      |              |
| Methyl isocyanate                                     | 0.02                       | 0.05                 |              |
| Methyl mercaptan                                      | 0.5                        | 1                    | highly toxic |
| Methyl methacrylate                                   | 100                        | 410                  |              |
| Methyl oxirane                                        | 20                         |                      | carcinogen   |
| 4-Methyl-2-pentanol                                   | 25                         | 104                  |              |
| 4-Methyl-2-pentanone                                  | 50                         | 205                  |              |
| 2-Methyl-2,4-pentanediol                              | 25                         | 121                  |              |
| 2-Methyl-1-propanol                                   | 50                         | 152                  |              |
| 2-Methyl-2-propanol                                   | 100                        | 303                  |              |
| 2-Methyl-2-propenenitrile                             | 1                          | 2.7                  |              |
| <i>o</i> -Methylstyrene (also <i>m</i> -, <i>p</i> -) | 50                         |                      |              |
| Morpholine                                            | 20                         | 70                   |              |
| Naphthalene                                           | 10                         | 50                   |              |
| Nickel carbonyl [Ni(CO) <sub>4</sub> ]                | 0.05                       | 0.35                 | carcinogen   |
| Nicotine                                              |                            | 0.5                  |              |
| Nitric acid                                           | 2                          | 5                    |              |
| Nitric oxide                                          | 25                         | 30                   | highly toxic |
| Nitrobenzene                                          | 1                          | 5                    |              |
| <i>p</i> -Nitrochlorobenzene                          |                            | 1                    |              |
| Nitroethane                                           | 100                        | 310                  |              |
| Nitrogen dioxide                                      | 3                          |                      | highly toxic |
| Nitrogen trifluoride                                  | 10                         |                      |              |
| Nitrogen trioxide                                     | 10                         | 29                   | highly toxic |
| Nitroglycerine                                        | 0.2                        | 2                    |              |
| Nitromethane                                          | 100                        | 250                  |              |
| 1-Nitropropane                                        | 25                         | 90                   |              |
| 2-Nitropropane                                        | 10                         | 36                   |              |
| Nitrosyl chloride                                     |                            |                      | highly toxic |
| <i>o</i> -Nitrotoluene (also <i>m</i> -, <i>p</i> -)  | 2                          |                      |              |
| Nonane                                                | 200                        | 1050                 |              |
| Octachloronaphthalene                                 |                            | 0.1                  |              |
| Octane                                                | 300                        | 1450                 |              |
| Oxalic acid                                           |                            | 1                    |              |
| 2-Oxetanone                                           | 0.05                       |                      | carcinogen   |
| Oxygen difluoride                                     | 0.05                       | 0.1                  |              |
| Ozone                                                 | 0.1                        | 0.2                  |              |
| Parathion                                             |                            | 0.1                  |              |
| Pentaborane                                           | 0.005                      | 0.01                 |              |
| Pentachloronaphthalene                                |                            | 0.5                  |              |
| Pentachlorophenol                                     |                            | 0.5                  |              |
| Pentanal                                              | 50                         |                      |              |
| Pentane                                               | 600                        | 1770                 |              |
| 2-Pentanone                                           | 200                        | 700                  |              |
| 3-Pentanone                                           | 200                        | 700                  |              |
| Pentyl acetate                                        | 100                        | 530                  |              |
| Perchloroethylene                                     | 100                        | 670                  |              |
| Perchloromethyl mercaptan                             | 0.1                        | 0.8                  |              |
| Perchloryl fluoride                                   | 3                          | 14                   |              |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                  | Maximum allowable exposure |                      | Toxicity     |
|----------------------------|----------------------------|----------------------|--------------|
|                            | ppm                        | mg · m <sup>-3</sup> |              |
| Perfluoroacetone           | 0.1                        |                      |              |
| Phenol                     | 5                          | 19                   |              |
| p-Phenylenediamine         |                            | 0.1                  |              |
| Phenylhydrazine            | 0.1                        |                      | carcinogen   |
| Phosgene                   | 0.1                        | 0.4                  | highly toxic |
| Phosphine                  | 0.3                        | 0.4                  | highly toxic |
| Phosphoric acid            |                            | 1                    |              |
| Phosphorus pentachloride   |                            | 1                    |              |
| Phosphorus pentafluoride   |                            |                      | highly toxic |
| Phosphorus pentasulfide    |                            | 1                    |              |
| Phosphorus trichloride     | 0.5                        | 3                    |              |
| Phosphoryl chloride        | 0.1                        |                      |              |
| Phthalic anhydride         | 1                          | 6                    |              |
| Picric acid—skin           |                            | 0.1                  |              |
| Propane                    | 1000                       | 1800                 | low toxicity |
| Propanoic acid             | 10                         | 30                   |              |
| 1-Propanol                 | 200                        | 500                  |              |
| 2-Propanol                 | 400                        | 980                  |              |
| Propenal                   | 0.1                        |                      |              |
| Propenenitrile             | 2                          |                      | carcinogen   |
| Propenoic acid             | 2                          |                      |              |
| Propyl acetate             | 200                        | 835                  |              |
| Propyleneimine             | 2                          | 5                    | carcinogen   |
| Propylene oxide            | 100                        | 240                  | toxic        |
| Propyl nitrate             | 25                         | 110                  |              |
| Propyne                    | 1000                       | 1650                 |              |
| 2-Propyn-1-ol              | 1                          | 2.3                  |              |
| Pyridine                   | 5                          | 15                   |              |
| Quinone                    | 0.1                        | 0.4                  |              |
| Selenium compounds (as Se) |                            | 0.2                  |              |
| Selenium hexafluoride      | 0.05                       | 0.4                  |              |
| Silane                     | 5                          | 7                    | highly toxic |
| Silicon tetrafluoride      |                            |                      | highly toxic |
| Stibine                    | 0.1                        |                      |              |
| Stoddard solvent           | 100                        | 575                  |              |
| Strychnine                 |                            | 0.15                 |              |
| Styrene                    | 50                         | 213                  | carcinogen   |
| Sulfur dioxide             | 2                          |                      | highly toxic |
| Sulfur hexafluoride        | 1000                       | 6000                 | low toxicity |
| Sulfuric acid              |                            | 1                    |              |
| Sulfur monochloride        | 1                          | 6                    |              |
| Sulfur pentafluoride       | 0.01                       |                      |              |
| Sulfur tetrafluoride       | 0.1                        | 0.4                  |              |
| Sulfuryl fluoride          | 5                          | 20                   | highly toxic |
| Tellurium hexafluoride     | 0.02                       | 0.2                  |              |
| Terphenyls                 | 1                          | 9                    |              |
| 1,1,2,2-Tetrabromoethane   | 1                          | 14                   |              |

**TABLE 11.49** TLV Concentration Limits for Gases and Vapors (*Continued*)

| Substance                                                     | Maximum allowable exposure |                      | Toxicity            |
|---------------------------------------------------------------|----------------------------|----------------------|---------------------|
|                                                               | ppm                        | mg · m <sup>-3</sup> |                     |
| Tetrabromomethane                                             | 0.1                        |                      |                     |
| 1,1,1,2-Tetrachloro-2,2-difluoroethane                        | 500                        | 4170                 |                     |
| 1,1,2,2-Tetrachloro-1,2-difluoroethane                        | 500                        | 4170                 |                     |
| 1,1,2,2-Tetrachloroethane                                     | 1                          | 6.9                  | carcinogen          |
| Tetrachloroethylene                                           | 25                         | 170                  | carcinogen          |
| Tetrachloromethane                                            | 5                          | 31                   | carcinogen          |
| 1,2,3,4-Tetrachloronaphthalene                                |                            | 2                    |                     |
| Tetraethyllead (as Pb)                                        |                            | 0.100                |                     |
| Tetrafluoromethane                                            |                            |                      | low toxicity        |
| Tetrahydrofuran                                               | 200                        | 590                  |                     |
| Tetramethyllead (as Pb)                                       |                            | 0.150                |                     |
| Tetramethylsuccinonitrile                                     | 0.5                        | 3                    |                     |
| Tetranitromethane                                             | 1                          | 8                    |                     |
| Thionyl chloride                                              | 1                          |                      |                     |
| Thiram                                                        |                            | 5                    |                     |
| Toluene                                                       | 50                         | 188                  |                     |
| Toluene-2,4-diisocyanate                                      | 0.02                       | 0.14                 |                     |
| <i>o</i> -Toluidine (also <i>m</i> -, <i>p</i> -)             | 2                          | 8.8                  |                     |
| Tribromomethane                                               | 0.5                        | 5.2                  |                     |
| Tributyl phosphate                                            | 0.2                        | 2.2                  |                     |
| 1,2,4-Trichlorobenzene                                        | 5                          |                      |                     |
| 1,1,1-Trichloroethane                                         | 350                        | 1910                 |                     |
| 1,1,2-Trichloroethane                                         | 10                         | 55                   | carcinogen          |
| Trichloroethylene                                             | 50                         | 270                  | carcinogen          |
| Trichlorofluoromethane                                        | 1000                       | 5600                 |                     |
| Trichloromethane                                              | 10                         | 49                   | carcinogen          |
| 1,2,3-Trichloropropane                                        | 10                         | 60                   |                     |
| 1,1,2-Trichlorotrifluoroethane                                | 1000                       |                      |                     |
| Tri- <i>o</i> -cresol phosphate (also <i>m</i> -, <i>p</i> -) |                            | 0.1                  |                     |
| Triethanolamine                                               | 0.5                        |                      |                     |
| Triethylamine                                                 | 1                          |                      |                     |
| Trifluorobromomethane (Freon 13B1)                            | 1000                       | 6100                 |                     |
| 1,1,2-Trifluorotrchloroethane                                 | 1000                       | 7600                 |                     |
| Triiodomethane                                                | 0.6                        |                      |                     |
| Trimethylamine                                                | 5                          | 12                   | highly toxic        |
| 1,2,3-Trimethylbenzene                                        | 25                         | 123                  |                     |
| 1,2,4-Trimethylbenzene (pseudocumene)                         | 25                         | 123                  |                     |
| 1,3,5-Trimethylbenzene (mesitylene)                           | 25                         | 123                  |                     |
| Trinitrotoluene (TNT)                                         |                            | 1.5                  |                     |
| Triphenyl phosphate                                           |                            | 3                    |                     |
| Turpentine                                                    | 100                        | 560                  |                     |
| Vinyl acetate                                                 | 10                         | 35                   | carcinogen          |
| Vinyl methyl ether                                            |                            |                      | probably anesthetic |
| Warfarin                                                      |                            | 0.1                  |                     |
| <i>o</i> -Xylene (also <i>m</i> -, <i>p</i> -)                | 100                        | 434                  |                     |
| 2,3-Xylydine (also 2,4-, 2,5-, 2,6-, 3,4-, 3,5-)              | 0.5                        | 2.5                  |                     |

**TABLE 11.50** Some Common Reactive and Incompatible Chemicals

| Chemical             | Keep out of contact with                                                                                                                                                                                                                                                                                                                                                       |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Acetic acid          | Chromium(VI) oxide, chlorosulfonic acid, ethylene glycol, ethyleneimine, hydroxyl compounds, nitric acid, oleum, perchloric acid, peroxides, permanganates, potassium <i>tert</i> -butoxide, $\text{PCl}_3$                                                                                                                                                                    |
| Acetylene            | Bromine, chlorine, brass, copper and copper salts, fluorine, mercury and mercury salts, nitric acid, silver and silver salts, alkali hydrides, potassium metal                                                                                                                                                                                                                 |
| Alkali metals        | Moisture, acetylene, metal halides, ammonium salts, oxygen and oxidizing agents, halogens, carbon tetrachloride, carbon, carbon dioxide, carbon disulfide, chloroform, chlorinated hydrocarbons, ethylene oxide, boric acid, sulfur, tellurium                                                                                                                                 |
| Aluminum             | Chlorinated hydrocarbons, halogens, steam                                                                                                                                                                                                                                                                                                                                      |
| Ammonia, anhydrous   | Mercury, halogens, hypochlorites, chlorites, chlorine(I) oxide, hydrofluoric acid (anhydrous), hydrogen peroxide, chromium(VI) oxide, nitrogen dioxide, chromyl(VI) chloride, sulfinyl chloride, magnesium perchlorate, peroxodisulfates, phosphorus pentoxide, acetaldehyde, ethylene oxide, acrolein, gold(III) chloride                                                     |
| Ammonium nitrate     | Acids, metal powders, flammable liquids, chlorates, nitrites, sulfur, finely divided organic or combustible materials, perchlorates, urea                                                                                                                                                                                                                                      |
| Ammonium perchlorate | Hot copper tubing, sugar, finely divided organic or combustible materials, potassium periodate and permanganate, powdered metals, carbon, sulfur                                                                                                                                                                                                                               |
| Aniline              | Nitric acid, peroxides, oxidizing materials, acetic anhydride, chlorosulfonic acid, oleum, ozone                                                                                                                                                                                                                                                                               |
| Benzoyl peroxide     | Direct sunlight, sparks and open flames, shock and friction, acids, alcohols, amines, ethers, reducing agents, polymerization catalysts, metallic naphthenates                                                                                                                                                                                                                 |
| Bromine              | Ammonia, carbides, dimethylformamide, fluorine, ozone, olefins, reducing materials including many metals, phosphine, silver azide                                                                                                                                                                                                                                              |
| Calcium carbide      | Moisture, selenium, silver nitrate, sodium peroxide, tin(II) chloride, potassium hydroxide plus chlorine, HCl gas, magnesium                                                                                                                                                                                                                                                   |
| Carbon, activated    | Calcium hypochlorite, all oxidizing agents, unsaturated oils                                                                                                                                                                                                                                                                                                                   |
| Chlorates            | Ammonium salts, acids, metal powders, sulfur, finely divided organic or combustible materials, cyanides, metal sulfides, manganese dioxide, sulfur dioxide, organic acids                                                                                                                                                                                                      |
| Chlorine             | Ammonia, acetylene, alcohols, alkanes, benzene, butadiene, carbon disulfide, dibutyl phthalate, ethers, fluorine, glycerol, hydrocarbons, hydrogen, sodium carbide, finely divided metals, metal acetylides and carbides, nitrogen compounds, nonmetals, nonmetal hydrides, phosphorus compounds, polychlorobiphenyl, silicones, steel, sulfides, synthetic rubber, turpentine |
| Chlorine dioxide     | Ammonia, carbon monoxide, hydrogen, hydrogen sulfide, methane, mercury, nonmetals, phosphine, phosphorus pentachloride                                                                                                                                                                                                                                                         |
| Chlorites            | Ammonia, organic matter, metals                                                                                                                                                                                                                                                                                                                                                |
| Chloroform           | Aluminum, magnesium, potassium, sodium, aluminum chloride, ethylene, powerful oxidants                                                                                                                                                                                                                                                                                         |
| Chlorosulfonic acid  | Saturated and unsaturated acids, acid anhydrides, nitriles, acrolein, alcohols, ammonia, esters, HCl, HF, ketones, hydrogen peroxide, metal powders, nitric acid, organic materials, water                                                                                                                                                                                     |
| Chromic(VI) acid     | Acetic acid, acetic anhydride, acetone, alcohols, alkali metals, ammonia, dimethylformamide, camphor, glycerol, hydrogen sulfide, phosphorus, pyridine, selenium, sulfur, turpentine, flammable liquids in general                                                                                                                                                             |
| Cobalt               | Acetylene, hydrazinium nitrate, oxidants                                                                                                                                                                                                                                                                                                                                       |
| Copper               | Acetylene and alkynes, ammonium nitrate, azides, bromates, chlorates, iodates, chlorine, ethylene oxide, fluorine, peroxides, hydrogen sulfide, hydrazinium nitrate                                                                                                                                                                                                            |

**TABLE 11.50** Some Common Reactive and Incompatible Chemicals (*Continued*)

| Chemical              | Keep out of contact with                                                                                                                                                                                           |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Copper(II) sulfate    | Hydroxylamine, magnesium                                                                                                                                                                                           |
| Cumene hydroperoxide  | Acids (inorganic or organic)                                                                                                                                                                                       |
| Cyanides              | Acids, water or steam, fluorine, magnesium, nitric acid and nitrates, nitrites                                                                                                                                     |
| Cyclohexanol          | Oxidants                                                                                                                                                                                                           |
| Cyclohexanone         | Hydrogen peroxide, nitric acid                                                                                                                                                                                     |
| Decaborane-14         | Dimethyl sulfoxide, ethers, halocarbons                                                                                                                                                                            |
| Diazomethane          | Alkali metals, calcium sulfate                                                                                                                                                                                     |
| 1,1-Dichloroethylene  | Air, chlorotrifluoroethylene, ozone, perchloryl fluoride                                                                                                                                                           |
| Dimethylformamide     | Halocarbons, inorganic and organic nitrates, bromine, chromium(VI) oxide, aluminum trimethyl, phosphorus trioxide                                                                                                  |
| 1,1-Dimethylhydrazine | Air, hydrogen peroxide, nitric acid, nitrous oxide                                                                                                                                                                 |
| Dimethylsulfoxide     | Acyl and aryl halides, boron compounds, bromomethane, nitrogen dioxide, magnesium perchlorate, periodic acid, silver difluoride, sodium hydride, sulfur trioxide                                                   |
| Dinitrobenzenes       | Nitric acid                                                                                                                                                                                                        |
| Dinitrotoluenes       | Nitric acid                                                                                                                                                                                                        |
| 1,4-Dioxane           | Silver perchlorate                                                                                                                                                                                                 |
| Esters                | Nitrates                                                                                                                                                                                                           |
| Ethylamine            | Cellulose, oxidizers                                                                                                                                                                                               |
| Ethers                | Oxidizing materials, boron triiodide                                                                                                                                                                               |
| Ethylene              | Aluminum trichloride, carbon tetrachloride, chlorine, nitrogen oxides, tetrafluoroethylene                                                                                                                         |
| Ethylene oxide        | Acids and bases, alcohols, air, 1,3-nitroaniline, aluminum chloride, aluminum oxide, ammonia, copper, iron chlorides and oxides, magnesium perchlorate, mercaptans, potassium, tin chlorides, alkane thiols        |
| Ethyl ether           | Liquid air, chlorine, chromium(VI) oxide, lithium aluminum hydride, ozone, perchloric acid, peroxides                                                                                                              |
| Ethyl sulfate         | Oxidizing materials, water                                                                                                                                                                                         |
| Flammable liquids     | Ammonium nitrate, chromic acid, the halogens, hydrogen peroxide, nitric acid                                                                                                                                       |
| Fluorine              | Isolate from everything; only lead and nickel resist prolonged attack                                                                                                                                              |
| Formamide             | Iodine, pyridine, sulfur trioxide                                                                                                                                                                                  |
| Freon 113             | Aluminum, barium, lithium, samarium, NaK alloy, titanium                                                                                                                                                           |
| Glycerol              | Acetic anhydride, hypochlorites, chromium(VI) oxide, perchlorates, alkali peroxides, sodium hydride                                                                                                                |
| Hydrazine             | Alkali metals, ammonia, chlorine, chromates and dichromates, copper salts, fluorine, hydrogen peroxide, metallic oxides, nickel, nitric acid, liquid oxygen, zinc diethyl                                          |
| Hydrides              | Powerful oxidizing agents, moisture                                                                                                                                                                                |
| Hydrocarbons          | Halogens, chromium(VI) oxide, peroxides                                                                                                                                                                            |
| Hydrogen              | Halogens, lithium, oxidants, lead trifluoride                                                                                                                                                                      |
| Hydrogen bromide      | Fluorine, iron(III) oxide, ammonia, ozone                                                                                                                                                                          |
| Hydrogen chloride     | Acetic anhydride, aluminum, 2-aminoethanol, ammonia, chlorosulfonic acid, ethylenediamine, fluorine, metal acetylides and carbides, oleum, perchloric acid, potassium permanganate, sodium, sulfuric acid          |
| Hydrogen fluoride     | Acetic anhydride, 2-aminoethanol, ammonia, arsenic trioxide, chlorosulfonic acid, ethylenediamine, ethyleneimine, fluorine, HgO, oleum, phosphorus trioxide, propylene oxide, sodium, sulfuric acid, vinyl acetate |
| Hydrogen iodide       | Fluorine, nitric acid, ozone, metals                                                                                                                                                                               |
| Hydrogen peroxide     | Copper, chromium, iron, most metals or their salts, alcohols, acetone, organic materials, flammable liquids, combustible materials                                                                                 |
| Hydrogen selenide     | Hydrogen peroxide, nitric acid                                                                                                                                                                                     |
| Hydrogen sulfide      | Fuming nitric acid, oxidizing gases, peroxides                                                                                                                                                                     |

**TABLE 11.50** Some Common Reactive and Incompatible Chemicals (*Continued*)

| Chemical                  | Keep out of contact with                                                                                                                                                                                                                          |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Hydroquinone              | Sodium hydroxide                                                                                                                                                                                                                                  |
| Hydroxylamine             | Barium oxide and peroxide, carbonyls, chlorine, copper(II) sulfate, dichromates, lead dioxide, phosphorus trichloride and pentachloride, permanganates, pyridine, sodium, zinc                                                                    |
| Hypochlorites, salts of   | Urea, amines, anthracene, carbon, carbon tetrachloride, ethanol, glycerol, mercaptans, organic sulfides, sulfur, thiols                                                                                                                           |
| Indium                    | Acetonitrile, nitrogen dioxide, mercury(II) bromide, sulfur                                                                                                                                                                                       |
| Iodine                    | Acetaldehyde, acetylene, aluminum, ammonia (aqueous or anhydrous), antimony, bromine pentafluoride, carbides, cesium oxide, chlorine, ethanol, fluorine, formamide, lithium, magnesium, phosphorus, pyridine, silver azide, sulfur trioxide       |
| Iodine monochloride       | Aluminum foil, organic matter, metal sulfides, phosphorus, potassium, rubber, sodium                                                                                                                                                              |
| Iodoform                  | Acetone, lithium, mercury(II) oxide, mercury(I) chloride, silver nitrate                                                                                                                                                                          |
| Iodomethane               | Silver chloride, sodium                                                                                                                                                                                                                           |
| Iron disulfide            | Water, powdered pyrites                                                                                                                                                                                                                           |
| Isothiourea               | Acrylaldehyde, hydrogen peroxide, nitric acid                                                                                                                                                                                                     |
| Ketones                   | Aldehydes, nitric acid, perchloric acid                                                                                                                                                                                                           |
| Lactonitrile              | Oxidizing materials                                                                                                                                                                                                                               |
| Lead                      | Ammonium nitrate, chlorine trifluoride, hydrogen peroxide, sodium azide and carbide, zirconium, oxidants                                                                                                                                          |
| Lead(II) azide            | Calcium stearate, copper, zinc, brass, carbon disulfide                                                                                                                                                                                           |
| Lead chromate             | Iron hexacyanoferrate(4-)                                                                                                                                                                                                                         |
| Lead dioxide              | Aluminum carbide, hydrogen peroxide, hydrogen sulfide, hydroxylamine, nitroalkanes, nitrogen compounds, nonmetal halides, peroxyformic acid, phosphorus, phosphorus trichloride, potassium, sulfur, sulfur dioxide, sulfides, tungsten, zirconium |
| Lead(II) oxide            | Chlorinated rubber, chlorine, ethylene, fluorine, glycerol, metal acetylides, perchloric acid                                                                                                                                                     |
| Lead(II,IV) oxide         | Same as for lead dioxide                                                                                                                                                                                                                          |
| Lithium hydride           | Nitrous oxide, oxygen                                                                                                                                                                                                                             |
| Magnesium                 | Air, beryllium fluoride, ethylene oxide, halogens, halocarbons, HI, metal cyanides, metal oxides, metal oxosalts, methanol, oxidants, peroxides, sulfur, tellurium                                                                                |
| Maleic anhydride          | Alkali metals, amines, KOH, NaOH, pyridine                                                                                                                                                                                                        |
| Manganese dioxide         | Aluminum, hydrogen sulfide, oxidants, potassium azide, hydrogen peroxide, peroxosulfuric acid, sodium peroxide                                                                                                                                    |
| Mercaptans                | Powerful oxidizers                                                                                                                                                                                                                                |
| Mercury                   | Acetylenic compounds, chlorine, fulminic acid, ammonia, ethylene oxide, metals, methyl azide, oxidants, tetracarbonylnickel                                                                                                                       |
| Mercury(II) cyanide       | Fluorine, hydrogen cyanide, magnesium, sodium nitrite                                                                                                                                                                                             |
| Mercury(I) nitrate        | Phosphorus                                                                                                                                                                                                                                        |
| Mercury(II) nitrate       | Acetylene, aromatics, ethanol, hypophosphoric acid, phosphine, unsaturated organic compounds                                                                                                                                                      |
| Mercury(II) oxide         | Chlorine, hydrazine hydrate, hydrogen peroxide, hypophosphorous acid, magnesium, phosphorus, sulfur, butadiene, hydrocarbons, methanethiol                                                                                                        |
| Mesityl oxide             | 2-Aminoethanol, chlorosulfonic acid, nitric acid, ethylenediamine, sulfuric acid                                                                                                                                                                  |
| Methanol                  | Beryllium dihydride, chloroform, oxidants, potassium <i>tert</i> -butoxide                                                                                                                                                                        |
| Methylamine               | Nitromethane                                                                                                                                                                                                                                      |
| <i>N</i> -Methylformamide | Benzenesulfonyl chloride                                                                                                                                                                                                                          |
| Methyl isobutyl ketone    | Potassium <i>tert</i> -butoxide                                                                                                                                                                                                                   |

**TABLE 11.50** Some Common Reactive and Incompatible Chemicals (*Continued*)

| Chemical                 | Keep out of contact with                                                                                                                                                                                                                    |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Methyl methacrylate      | Air, benzoyl peroxide                                                                                                                                                                                                                       |
| 4-Methylnitrobenzene     | Sulfuric acid, tetranitromethane                                                                                                                                                                                                            |
| 2-Methylpyridine         | Hydrogen peroxide, iron(II) sulfate, sulfuric acid                                                                                                                                                                                          |
| Methylsodium             | 4-Chloronitrobenzene                                                                                                                                                                                                                        |
| Molybdenum trioxide      | Chlorine trifluoride, interhalogens, metals                                                                                                                                                                                                 |
| Naphthalene              | Chromium trioxide, dinitrogen pentaoxide                                                                                                                                                                                                    |
| 2-Naphthol               | Antipyrine, camphor, phenol, iron(III) salts, menthol, oxidizing materials, permanganates, urethane                                                                                                                                         |
| Neodymium                | Phosphorus                                                                                                                                                                                                                                  |
| Nickel                   | Aluminum, aluminum(III) chloride, ethylene, 1,4-dioxan, hydrogen, methanol, nonmetals, oxidants, sulfur compounds                                                                                                                           |
| Nickel carbonyl          | Air, bromine, oxidizing materials                                                                                                                                                                                                           |
| Niobium                  | Bromine trifluoride, chlorine, fluorine                                                                                                                                                                                                     |
| Nitrates                 | Aluminum, BP, cyanides, esters, phosphorus, tin(II) chloride, sodium hypophosphite, thiocyanates                                                                                                                                            |
| Nitric acid, fuming      | Organic matter, nonmetals, most metals, ammonia, chlorosulfonic acid, chromium trioxide, cyanides, dichromates, hydrazines, hydrides, HCN, HI, hydrogen sulfide, sulfur dioxide, sulfur halides, sulfuric acid, flammable liquids and gases |
| Nitric oxide             | Aluminum, BaO, boron, carbon disulfide, chromium, many chlorinated hydrocarbons, fluorine, hydrocarbons, ozone, phosphine, phosphorus, hydrazine, acetic anhydride, ammonia, chloroform, Fe, K, Mg, Mn, Na, sulfur                          |
| Nitrites                 | Organic nitrites in contact with ammonium salts, cyanides                                                                                                                                                                                   |
| Nitrobenzene             | Nitric acid, nitrous oxide, silver perchlorate                                                                                                                                                                                              |
| Nitroethane              | Hydroxides, hydrocarbons, metal oxides                                                                                                                                                                                                      |
| Nitrogen trichloride     | Ammonia, As, hydrogen sulfide, nitrogen dioxide, organic matter, ozone, phosphine, phosphorus, KCN, KOH, Se, dibutyl ether                                                                                                                  |
| Nitrogen dioxide         | Cyclohexane, fluorine, formaldehyde, alcohols, nitrobenzene, petroleum, toluene                                                                                                                                                             |
| Nitrogen triiodide       | Acids, bromine, chlorine, hydrogen sulfide, ozone                                                                                                                                                                                           |
| $\alpha$ -Nitroguanidine | Complex salts of mercury and silver                                                                                                                                                                                                         |
| Nitromethane             | Acids, alkylmetal halides, hydroxides, hydrocarbons, organic amines, formaldehyde, nitric acid, perchlorates                                                                                                                                |
| 1-Nitropropane           | See under Nitromethane; chlorosulfonic acid, oleum                                                                                                                                                                                          |
| Nitrosyl fluoride        | Haloalkenes, metals, nonmetals                                                                                                                                                                                                              |
| Nitrosyl perchlorate     | Acetones, amines, diethyl ether, metal salts, organic materials                                                                                                                                                                             |
| Nitrourea                | Mercury(II) and silver salts                                                                                                                                                                                                                |
| Nitrous acid             | Phosphine, phosphorus trichloride, silver nitrate, semicarbazone                                                                                                                                                                            |
| Nitryl chloride          | Ammonia, sulfur trioxide, tin(IV) bromide and iodide                                                                                                                                                                                        |
| Oxalic acid              | Furfuryl alcohol, silver, mercury, sodium chlorate, sodium chlorite, sodium hypochlorite                                                                                                                                                    |
| Oxygen                   | Acetaldehyde, acetone, alcohols, alkali metals, alkaline earth metals, Al-Ti alloys, ether, carbon disulfide, halocarbons, hydrocarbons, metal hydrides, 1,3,5-trioxane                                                                     |
| Ozone                    | Alkenes, aromatic compounds, bromine, diethyl ether, ethylene, HBr, HI, nitric oxide, nitrogen dioxide, rubber, stibine                                                                                                                     |
| Palladium                | Arsenic, carbon, ozonides, sulfur, sodium tetrahydridoborate                                                                                                                                                                                |
| Paraformaldehyde         | Liquid oxygen                                                                                                                                                                                                                               |
| Paraldehyde              | Alkalies, HCN, iodides, nitric acid, oxidizers                                                                                                                                                                                              |
| Pentaborane-9            | Dimethylsulfoxide                                                                                                                                                                                                                           |
| Pentacarbonyliron        | Acetic acid, nitric oxide, transition metal halides, water, zinc                                                                                                                                                                            |



**TABLE 11.50** Some Common Reactive and Incompatible Chemicals (*Continued*)

| Chemical                        | Keep out of contact with                                                                                                                                                                                                                                                                                                     |
|---------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 2-Pentanone                     | Bromine trifluoride                                                                                                                                                                                                                                                                                                          |
| 3-Pentanone                     | Hydrogen peroxide, nitric acid                                                                                                                                                                                                                                                                                               |
| Perchlorates                    | Carbonaceous materials, finely divided metals particularly magnesium and aluminum, sulfur, benzene, olefins, ethanol, sulfur, sulfuric acid                                                                                                                                                                                  |
| Perchloric acid                 | Acetic acid, acetic anhydride, alcohols, antimony compounds, azo pigments, bismuth and its alloys, methanol, carbonaceous materials, carbon tetrachloride, cellulose, dehydrating agents, diethyl ether, glycols and glycolethers, HCl, HI, hypophosphites, ketones, nitric acid, pyridine, steel, sulfoxides, sulfuric acid |
| Permanganates                   | All reducing agents, organic materials                                                                                                                                                                                                                                                                                       |
| Peroxides                       | Reducing agents, organic materials, thiocyanates                                                                                                                                                                                                                                                                             |
| Peroxoacetic acid               | Acetic anhydride, olefins, organic matter                                                                                                                                                                                                                                                                                    |
| Peroxybenzoic acid              | Olefins, reducing materials                                                                                                                                                                                                                                                                                                  |
| Peroxoformic acid               | Metals and nonmetals, organic materials                                                                                                                                                                                                                                                                                      |
| Peroxyosulfuric acid            | Acetone, alcohols, aromatic compounds, catalysts                                                                                                                                                                                                                                                                             |
| Phenol                          | Butadiene, peroxodisulfuric acid, peroxosulfuric acid, aluminum chloride plus nitrobenzene                                                                                                                                                                                                                                   |
| Phenylhydrazine                 | Lead dioxide, oxidizers                                                                                                                                                                                                                                                                                                      |
| Phosgene                        | Aluminum, alkali metals, 2-propanol                                                                                                                                                                                                                                                                                          |
| Phosphine                       | Air, boron trichloride, bromine, chlorine, nitric acid, nitrogen oxides, nitrous acid, oxygen, silver nitrate                                                                                                                                                                                                                |
| Phosphorus pentachloride        | Aluminum, chlorine, chlorine dioxide, chlorine trioxide, fluorine, magnesium oxide, nitrobenzene, diphosphorus trioxide, potassium, sodium, urea, water                                                                                                                                                                      |
| Phosphorus pentafluoride        | Water or steam                                                                                                                                                                                                                                                                                                               |
| Phosphorus pentasulfide         | Air, alcohols, water                                                                                                                                                                                                                                                                                                         |
| Phosphorus pentoxide            | Formic acid, HF, inorganic bases, metals, oxidants, water                                                                                                                                                                                                                                                                    |
| Phosphorus, red                 | Organic materials                                                                                                                                                                                                                                                                                                            |
| Phosphorus tribromide           | Potassium, ruthenium tetroxide, sodium, water                                                                                                                                                                                                                                                                                |
| Phosphorus trichloride          | Acetic acid, aluminum, chromyl dichloride, dimethylsulfoxide, hydroxylamine, lead dioxide, nitric acid, nitrous acid, organic matter, potassium, sodium water                                                                                                                                                                |
| Phosphorus, white               | Air, oxidants of all types, halogens, metals                                                                                                                                                                                                                                                                                 |
| Phosphoryl chloride             | Carbon disulfide, <i>N,N</i> -dimethylformamide, 2,5-dimethylpyrrole, 2,6-dimethylpyridine 1-oxide, dimethylsulfoxide, water, zinc                                                                                                                                                                                           |
| Phthalic acid                   | Nitric acid, sodium nitrite                                                                                                                                                                                                                                                                                                  |
| Piperazine                      | Oxidizers                                                                                                                                                                                                                                                                                                                    |
| Platinum                        | Acetone, arsenic, hydrazine, lithium, peroxosulfuric acid, phosphorus, selenium, tellurium                                                                                                                                                                                                                                   |
| Potassium                       | <i>See under</i> Alkali metals                                                                                                                                                                                                                                                                                               |
| Potassium <i>tert</i> -butoxide | Organic compounds, sulfuric acid                                                                                                                                                                                                                                                                                             |
| Potassium hydride               | Air, chlorine, acetic acid, acrolein, acrylonitrile, maleic anhydride, nitroparaffins, <i>N</i> -nitrosomethylurea, tetrahydrofuran, water                                                                                                                                                                                   |
| Potassium perchlorate           | Aluminum plus magnesium, carbon, nickel plus titanium, reducing agents, sulfur, sulfuric acid                                                                                                                                                                                                                                |
| Potassium permanganate          | Organic or readily oxidizable materials                                                                                                                                                                                                                                                                                      |
| Potassium sodium alloy          | Air, carbon dioxide, carbon disulfide, halocarbons, metal oxides                                                                                                                                                                                                                                                             |
| 2-Propyn-1-ol                   | Alkali metals, mercury(II) sulfate, oxidizing materials, phosphorus pentoxide, sulfuric acid                                                                                                                                                                                                                                 |
| Pyridine                        | Chlorosulfonic acid, chromium trioxide, formamide, maleic anhydride, nitric acid, oleum, perchromates, silver perchlorate, sulfuric acid                                                                                                                                                                                     |
| Pyrrolidine                     | Oxidizing materials                                                                                                                                                                                                                                                                                                          |

**TABLE 11.50** Some Common Reactive and Incompatible Chemicals (*Continued*)

| Chemical              | Keep out of contact with                                                                                                                                                                                                |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Quinoline             | Dinitrogen tetroxide, linseed oil, maleic anhydride, thionyl chloride                                                                                                                                                   |
| Salicylic acid        | Iodine, iron salts, lead acetate                                                                                                                                                                                        |
| Silicon               | Alkali carbonates, calcium, chlorine, cobalt(II) fluoride, manganese trifluoride, oxidants, silver fluoride, sodium-potassium alloy                                                                                     |
| Silver                | Acetylene, ammonium compounds, ethyleneimine, hydrogen peroxide, oxalic acid, sulfuric acid, tartaric acid                                                                                                              |
| Sodium                | See under Alkali metals                                                                                                                                                                                                 |
| Sodium peroxide       | Glacial acetic acid, acetic anhydride, aniline, benzene, benzaldehyde, carbon disulfide, diethyl ether, ethanol or methanol, ethylene glycol, ethyl acetate, furfural, glycerol, metals, methyl acetate, organic matter |
| Sulfides              | Acids, powerful oxidizers, moisture                                                                                                                                                                                     |
| Sulfur                | Oxidizing materials, halogens                                                                                                                                                                                           |
| Sulfur dioxide        | Halogens, metal oxides, polymeric tubing, potassium chlorate, sodium hydride                                                                                                                                            |
| Sulfuric acid         | Chlorates, metals, HCl, organic materials, perchlorates, permanganates, water                                                                                                                                           |
| Sulfuryl dichloride   | Alkalis, diethyl ether, dimethylsulfoxide, dinitrogen tetroxide, lead dioxide, phosphorus                                                                                                                               |
| Tellurium             | Halogens, metals                                                                                                                                                                                                        |
| Tetrahydrofuran       | Tetrahydroaluminates, KOH, NaOH                                                                                                                                                                                         |
| Tetranitroaniline     | Reducing materials                                                                                                                                                                                                      |
| Tetranitromethane     | Aluminum, cotton, aromatic nitro compounds, hydrocarbons, cotton, toluene                                                                                                                                               |
| Thiocyanates          | Chlorates, nitric acid, peroxides                                                                                                                                                                                       |
| Thionyl chloride      | Ammonia, dimethylsulfoxide, linseed oil, quinoline, sodium                                                                                                                                                              |
| Thiophene             | Nitric acid                                                                                                                                                                                                             |
| Thymol                | Acetanilide, antipyrine, camphor, chlorohydrate, menthol, quinine sulfate, urethane                                                                                                                                     |
| Tin(II) chloride      | Boron trifluoride, ethylene oxide, hydrazine hydrate, nitrates, Na, K, hydrogen peroxide                                                                                                                                |
| Tin(IV) chloride      | Alkyl nitrates, ethylene oxide, K, Na turpentine                                                                                                                                                                        |
| Titanium              | Aluminum, boron trifluoride, carbon dioxide, CuO, halocarbons, halogens, PbO, nitric acid, potassium chlorate, potassium nitrate, potassium permanganate, steam at high temperatures, water                             |
| Toluene               | Sulfuric plus nitric acids, nitrogen dioxide, silver perchlorate, uranium hexafluoride                                                                                                                                  |
| Toluidines            | Nitric acid                                                                                                                                                                                                             |
| 2,4,6-Trinitrotoluene | Sodium dichromate, sulfuric acid                                                                                                                                                                                        |
| 1,3,5-Trioxane        | Oxidizing materials, acids                                                                                                                                                                                              |
| Urea                  | Sodium nitrite, phosphorus pentachloride                                                                                                                                                                                |
| Vinylidene chloride   | Chlorosulfonic acid, nitric acid, oleum                                                                                                                                                                                 |

TABLE 11.51 Chemicals Recommended for Refrigerated Storage

| A. Due to chemical decomposition or polymerization |                                        |
|----------------------------------------------------|----------------------------------------|
| Acetaldehyde                                       | Isoprene                               |
| Acrolein                                           | Lecithin                               |
| Adenosinetriphosphoric acid                        | Mercaptoacetic acid                    |
| Bromacetaldehyde, diethyl acetal                   | Methyl acrylate                        |
| Bromosuccinimide                                   | 2-Methyl-1-butene                      |
| 3-Buten-2-one                                      | Methylenedi-1,4-phenylene diisocyanate |
| tert-Butyl hydroperoxide                           | 4-Methyl-1-pentene                     |
| 2-Chlorocyclohexanone                              | α-Methylstyrene                        |
| Cupferron                                          | 1-Naphthyl isocyanate                  |
| 1,3-Cyclohexadiene                                 | 1-Pentene                              |
| 1,3-Dihydroxy-2-propanone                          | Isopentyl acetate                      |
| Divinylbenzene                                     | Pyruvic acid                           |
| Ethyl methacrylate, monomer                        | Styrene, stabilized                    |
| Glutathione                                        | Tetramethylsilane                      |
| Glycidol                                           | Thioacetamide                          |
| Histamine, base                                    | Veratraldehyde                         |
| Hydrocinnamaldehyde                                | Vitamin E (and the acetate)            |
| B. Due to flammability and high volatility         |                                        |
| Acetaldehyde                                       | Iodomethane                            |
| Bromoethane                                        | Isoprene                               |
| tert-Butylamine                                    | Isopropylamine                         |
| Carbon disulfide                                   | Methylal                               |
| 1-Chloropropane                                    | 2-Methylbutane                         |
| 3-Chloropropane                                    | 2-Methyl-2-butene                      |
| Cyclopentane                                       | Methyl formate                         |
| Diethyl ether                                      | Pentane                                |
| 2,2-Dimethylbutane                                 | Propylamine                            |
| Dimethyl sulfide                                   | Propylene oxide                        |
| Furan                                              | Trichlorosilane                        |

TABLE 11.52 Chemicals Which Polymerize or Decompose on Extended Refrigeration

|                                        |                   |
|----------------------------------------|-------------------|
| Formaldehyde                           | Sodium methoxide  |
| Hydrogen peroxide                      | Sodium nitrate    |
| Sodium chlorite [sodium chlorate (IV)] | Sodium peroxide   |
| Sodium chromate(VI)                    | Strontium nitrate |
| Sodium dithionite                      | Urea              |
| Sodium ethoxide                        |                   |

11.8 SIEVES AND SCREENS

TABLE 11.53 U.S. Standard Sieve Series

| Sieve no. | Sieve opening |        | Sieve no. | Sieve opening |        |
|-----------|---------------|--------|-----------|---------------|--------|
|           | mm            | inch   |           | mm            | inch   |
|           | 125           | 5.00   | 10        | 2.00          | 0.0787 |
|           | 106           | 4.24   | 12        | 1.70          | 0.0661 |
|           | 90            | 3.50   | 14        | 1.40          | 0.0555 |
|           | 75            | 3.00   | 16        | 1.18          | 0.0469 |
|           | 63            | 2.50   | 18        | 1.00          | 0.0394 |
|           | 53            | 2.12   | 20        | 0.850         | 0.0331 |
|           | 45            | 1.75   | 25        | 0.710         | 0.0278 |
|           | 37.5          | 1.50   | 30        | 0.600         | 0.0234 |
|           | 31.5          | 1.25   | 35        | 0.500         | 0.0197 |
|           | 26.5          | 1.06   | 40        | 0.425         | 0.0165 |
|           | 22.4          | 0.875  | 45        | 0.355         | 0.0139 |
|           | 19.0          | 0.75   | 50        | 0.300         | 0.0117 |
|           | 16.0          | 0.625  | 60        | 0.250         | 0.0098 |
|           | 13.2          | 0.530  | 70        | 0.212         | 0.0083 |
|           | 11.2          | 0.438  | 80        | 0.180         | 0.0070 |
|           | 9.5           | 0.375  | 100       | 0.150         | 0.0059 |
|           | 8.0           | 0.312  | 120       | 0.125         | 0.0049 |
|           | 6.7           | 0.265  | 140       | 0.106         | 0.0041 |
| 3.5       | 5.60          | 0.223  | 170       | 0.090         | 0.0035 |
| 4         | 4.75          | 0.187  | 200       | 0.075         | 0.0029 |
| 5         | 4.00          | 0.157  | 230       | 0.063         | 0.0025 |
| 6         | 3.35          | 0.132  | 270       | 0.053         | 0.0021 |
| 7         | 2.80          | 0.111  | 325       | 0.045         | 0.0017 |
| 8         | 2.36          | 0.0937 | 400       | 0.038         | 0.0015 |

Specifications are from ASTM E.11-81/ISO 565. The sieve numbers are the approximate number of openings per linear inch.

11.9 THERMOMETRY

11.9.1 Temperature and Its Measurement

The new international temperature scale, known as ITS-90, was adopted in September 1989. However, neither the definition of thermodynamic temperature nor the definition of the kelvin or the Celsius temperature scales has changed; it is the way in which we are to realize these definitions that has changed. The changes concern the recommended thermometers to be used in different regions of the temperature scale and the list of secondary standard fixed points. The changes in temperature determined using ITS-90 from the previous IPTS-68 are always less than 0.4 K, and almost always less than 0.2 K, over the range 0–1300 K.

The ultimate definition of thermodynamic temperature is in terms of  $pV$  (pressure  $\times$  volume) in a gas thermometer extrapolated to low pressure. The kelvin (K), the unit of thermodynamic temperature, is defined by specifying the temperature of one fixed point on the scale—the triple point

of water which is defined to be 273.16 K. The Celsius temperature scale ( $^{\circ}\text{C}$ ) is defined by the equation

$$^{\circ}\text{C} = \text{K} - 273.15$$

where the freezing point of water at 1 atm is 273.15 K.

The fixed points in the ITS-90 are given in Table 11.39. Platinum resistance thermometers are recommended for use between 14 K and 1235 K (the freezing point of silver), calibrated against the fixed points. Below 14 K either the vapor pressure of helium or a constant-volume gas thermometer is to be used. Above 1235 K radiometry is to be used in conjunction with the Planck radiation law,

$$L_{\lambda} = c_1 \lambda^{-5} (e^{c_2/\lambda T} - 1)^{-1}$$

where  $L_{\lambda}$  is the spectral radiance at wavelength  $\lambda$ . The first radiation constant,  $c_1$ , is  $3.741\,83 \times 10^{-16} \text{ W} \cdot \text{m}^2$  and the second radiation constant,  $c_2$ , has a value of  $0.014\,388 \text{ m} \cdot \text{K}$ .

**TABLE 11.54** Fixed Points in the ITS-90

| Fixed points                                              | $T$ , K  | $t$ , $^{\circ}\text{C}$ |
|-----------------------------------------------------------|----------|--------------------------|
| Triple point of hydrogen                                  | 13.8033  | − 259.3467               |
| Boiling point of hydrogen at 33 321.3 Pa                  | 17.035   | − 256.115                |
| Boiling point of hydrogen at 101 292 Pa                   | 20.27    | − 252.88                 |
| Triple point of neon                                      | 24.5561  | − 248.5939               |
| Triple point of oxygen                                    | 54.3584  | − 218.7916               |
| Triple point of argon                                     | 83.8058  | − 189.3442               |
| Triple point of mercury                                   | 234.3156 | − 38.8344                |
| Triple point of water                                     | 273.16   | 0.01                     |
| Melting point of gallium                                  | 302.9146 | 29.7646                  |
| Freezing point of indium                                  | 429.7458 | 156.5985                 |
| Freezing point of tin                                     | 505.078  | 231.928                  |
| Freezing point of zinc                                    | 692.677  | 419.527                  |
| Freezing point of aluminum                                | 933.473  | 660.323                  |
| Freezing point of silver                                  | 1234.93  | 961.78                   |
| Freezing point of gold                                    | 1337.33  | 1064.18                  |
| Freezing point of copper                                  | 1357.77  | 1084.62                  |
| Secondary reference points to extend the scale (IPTS-68): |          |                          |
| Freezing point of platinum                                | 2042     | 1769                     |
| Freezing point of rhodium                                 | 2236     | 1963                     |
| Freezing point of iridium                                 | 2720     | 2447                     |
| Melting point of tungsten                                 | 3660     | 3387                     |

11.10 THERMOCOUPLES

The thermocouple reference data in Tables 11.55 to 11.63 give the thermoelectric voltage in millivolts with the reference junction at  $0^{\circ}\text{C}$ . Note that the temperature for a given entry is obtained by adding the corresponding temperature in the top row to that in the left-hand column, regardless of whether the latter is positive or negative.

The noble metal thermocouples, Types B, R, and S, are all platinum or platinum-rhodium thermocouples and hence share many of the same characteristics. Metallic vapor diffusion at high temperatures can readily change the platinum wire calibration, hence platinum wires should only be used inside a nonmetallic sheath such as high-purity alumina.

Type B thermocouples (Table 11.56) offer distinct advantages of improved stability, increased mechanical strength, and higher possible operating temperatures. They have the unique advantage that the reference junction potential is almost immaterial, as long as it is between 0°C and 40°C. Type B is virtually useless below 50°C because it exhibits a double-value ambiguity from 0°C to 42°C.

Type E thermoelements (Table 11.57) are very useful down to about liquid hydrogen temperatures and may even be used down to liquid helium temperatures. They are the most useful of the commercially standardized thermocouple combinations for subzero temperature measurements because of their high Seebeck coefficient (58  $\mu\text{V}/^\circ\text{C}$ ), low thermal conductivity, and corrosion resistance. They also have the largest Seebeck coefficient (voltage response per degree Celsius) above 0°C of any of the standardized thermocouples which makes them useful for detecting small temperature changes. They are recommended for use in the temperature range from  $-250$  to  $871^\circ\text{C}$  in oxidizing or inert atmospheres. They should not be used in sulfurous, reducing, or alternately reducing and oxidizing atmospheres unless suitably protected with tubes. They should not be used in vacuum at high temperatures for extended periods of time.

Type J thermocouples (Table 11.58) are one of the most common types of industrial thermocouples because of the relatively high Seebeck coefficient and low cost. They are recommended for use in the temperature range from 0 to  $760^\circ\text{C}$  (but never above  $760^\circ\text{C}$  due to an abrupt magnetic transformation that can cause decalibration even when returned to lower temperatures). Use is permitted in vacuum and in oxidizing, reducing, or inert atmospheres, with the exception of sulfurous atmospheres above  $500^\circ\text{C}$ . For extended use above  $500^\circ\text{C}$ , heavy-gauge wires are recommended. They are not recommended for subzero temperatures. These thermocouples are subject to poor conformance characteristics because of impurities in the iron.

The Type K thermocouple (Table 11.59) is more resistant to oxidation at elevated temperatures than the Type E, J, or T thermocouple, and consequently finds wide application at temperatures above  $500^\circ\text{C}$ . It is recommended for continuous use at temperatures within the range  $-250$  to  $1260^\circ\text{C}$  in inert or oxidizing atmospheres. It should not be used in sulfurous or reducing atmospheres, or in vacuum at high temperatures for extended times.

The Type N thermocouple (Table 11.60) is similar to Type K but it has been designed to minimize some of the instabilities in the conventional Chromel-Alumel combination. Changes in the alloy content have improved the order/disorder transformations occurring at  $500^\circ\text{C}$  and a higher silicon content of the positive element improves the oxidation resistance at elevated temperatures.

The Type R thermocouple (Table 11.61) was developed primarily to match a previous platinum–10% rhodium British wire which was later found to have 0.34% iron impurity in the rhodium. Comments on Type S also apply to Type R.

The Type S thermocouple (Table 11.62) is so stable that it remains the standard for determining temperatures between the antimony point ( $630.74^\circ\text{C}$ ) and the gold point ( $1064.43^\circ\text{C}$ ). The other fixed point used is that of silver. The Type S thermocouple can be used from  $-50^\circ\text{C}$  continuously up to about  $1400^\circ\text{C}$ , and intermittently at temperatures up to the freezing point of platinum ( $1769^\circ\text{C}$ ). The thermocouple is most reliable when used in a clean oxidizing atmosphere, but may also be used in inert gaseous atmospheres or in a vacuum for short periods of time. It should not be used in reducing atmospheres, nor in those containing metallic vapor (such as lead or zinc), nonmetallic vapors (such as arsenic, phosphorus, or sulfur), or easily reduced oxides, unless suitably protected with nonmetallic protecting tubes.

The Type T thermocouple (Table 11.63) is popular for the temperature region below  $0^\circ\text{C}$  (but see under Type E). It can be used in vacuum, or in oxidizing, reducing, or inert atmospheres.

**TABLE 11.55** Thermoelectric Values in Millivolts at Fixed Points for Various Thermocouples

| <i>Abbreviations Used in the Table</i> |           |                   |         |         |         |        |         |         |         |
|----------------------------------------|-----------|-------------------|---------|---------|---------|--------|---------|---------|---------|
| FP, freezing point                     |           | BP, boiling point |         |         |         |        |         |         |         |
| NBP, normal boiling point              |           | TP, triple point  |         |         |         |        |         |         |         |
| Fixed point                            | °C        | Type B            | Type E  | Type J  | Type K  | Type N | Type R  | Type S  | Type T  |
| Helium NPB                             | −268.934  |                   | −9.8331 |         | −6.4569 | −4.345 |         |         | −6.2563 |
| Hydrogen TP                            | −259.347* |                   | −9.7927 |         | −6.4393 | −4.334 |         |         | −6.2292 |
| Hydrogen NBP                           | −252.88*  |                   | −9.7447 |         | −6.4167 | −4.321 |         |         | −6.1977 |
| Neon TP                                | −248.594* |                   | −9.7046 |         | −6.3966 | −4.271 |         |         | −6.1714 |
| Neon NBP                               | −246.048  |                   | −9.6776 |         | −6.3827 | −4.300 |         |         | −6.1536 |
| Oxygen TP                              | −218.792* |                   | −9.2499 |         | −6.1446 | −4.153 |         |         | −5.8730 |
| Nitrogen TP                            | −210.001  |                   | −9.0629 | −8.0957 | −6.0346 | −4.083 |         |         | −5.7533 |
| Nitrogen NBP                           | −195.802  |                   | −8.7168 | −7.7963 | −5.8257 | −3.947 |         |         | −5.5356 |
| Oxygen NBP                             | −182.962  |                   | −8.3608 | −7.4807 | −5.6051 | −3.802 |         |         | −5.3147 |
| Carbon dioxide SP                      | −78.474   |                   | −4.2275 | −3.7187 | −2.8696 | −1.939 |         |         | −2.7407 |
| Mercury TP                             | −38.834*  |                   | −2.1930 | −1.4849 |         | −0.985 | −0.1830 | −0.1895 | −1.4349 |
| Ice point                              | 0.000     | −0.000            | 0.000   | 0.000   | 0.000   | 0.000  | 0.000   | 0.000   | 0.000   |
| Diphenyl ether TP                      | 26.87     | −0.0024           | 1.6091  | 1.3739  | 1.076   | 0.698  | 0.1517  | 0.1537  | 1.0679  |
| Water BP                               | 100.00    | 0.0332            | 6.3171  | 5.2677  | 4.0953  | 2.774  | 0.6472  | 0.6453  | 4.2773  |

**TABLE 11.55** Thermoelectric Values in Millivolts at Fixed Points for Various Thermocouples (Continued)

| Abbreviations Used in the Table |          |                   |        |        |        |        |        |        |        |
|---------------------------------|----------|-------------------|--------|--------|--------|--------|--------|--------|--------|
| FP, freezing point              |          | BP, boiling point |        |        |        |        |        |        |        |
| NBP, normal boiling point       |          | TP, triple point  |        |        |        |        |        |        |        |
| Fixed point                     | °C       | Type B            | Type E | Type J | Type K | Type N | Type R | Type S | Type T |
| Benzoic acid TP                 | 122.37   | 0.0561            | 7.8468 | 6.4886 | 5.0160 | 3.446  | 0.8186 | 0.8129 | 5.3414 |
| Indium FP                       | 156.598* | 0.1019            | 10.260 | 8.3743 | 6.0404 | 4.508  | 1.0956 | 1.0818 | 7.0364 |
| Tin FP                          | 231.928* | 0.2474            | 15.809 | 12.552 | 9.4201 | 6.980  | 1.7561 | 1.7146 | 11.013 |
| Bismuth FP                      | 271.442  | 0.3477            | 18.821 | 14.743 | 11.029 | 8.336  | 2.1250 | 2.0640 | 13.219 |
| Cadmium FP                      | 321.108  | 0.4971            | 22.684 | 17.493 | 13.085 | 10.092 | 2.6072 | 2.5167 | 16.095 |
| Lead FP                         | 327.502  | 0.5182            | 23.186 | 17.846 | 13.351 | 10.322 | 2.6706 | 2.5759 | 16.473 |
| Mercury BP                      | 356.66   | 0.6197            | 25.489 | 19.456 | 14.571 |        | 2.9630 | 2.8483 | 18.218 |
| Zinc FP                         | 419.527* | 0.8678            | 30.513 | 22.926 | 17.223 |        | 3.6113 | 3.4479 |        |
| Cu-Al eutectic FP               | 548.23   | 1.4951            | 40.901 | 30.109 | 22.696 |        | 5.0009 | 4.7140 |        |
| Antimony FP                     | 630.74   | 1.9784            | 47.561 | 34.911 | 26.207 |        | 5.9331 | 5.5521 |        |
| Aluminum FP                     | 660.37   | 2.1668            | 49.941 | 36.693 | 27.461 |        | 6.2759 | 5.8591 |        |
| Silver FP                       | 961.93*  | 4.4908            | 73.495 | 55.669 | 39.779 |        | 10.003 | 9.1482 |        |
| Gold FP                         | 1064.43* | 5.4336            |        | 61.716 | 43.755 |        | 11.364 | 10.334 |        |
| Copper FP                       | 1084.5   | 5.6263            |        | 62.880 | 44.520 |        | 11.635 | 10.570 |        |
| Nickel FP                       | 1455     | 9.5766            |        |        |        |        | 16.811 | 15.034 |        |
| Cobalt FP                       | 1494     | 10.025            |        |        |        |        | 17.360 | 15.504 |        |
| Palladium FP                    | 1554     | 10.721            |        |        |        |        | 18.212 | 16.224 |        |
| Platinum FP                     | 1772     | 13.262            |        |        |        |        | 21.103 | 18.694 |        |

\* Defining fixed points of the International Temperature Scale of 1990 (ITS-90). Except for the triple points, the assigned values of temperature are for equilibrium states at a pressure of one standard atmosphere (101 325 Pa).



**TABLE 11.56** Type B Thermocouples: Platinum–30% Rhodium Alloy vs. Platinum–6% Rhodium Alloy*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C   | 0       | 10      | 20      | 30      | 40      | 50      | 60      | 70      | 80      | 90      |
|------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0    | 0.00    | −0.0019 | −0.0026 | −0.0021 | −0.0005 | 0.0023  | 0.0062  | 0.0112  | 0.0174  | 0.0248  |
| 100  | 0.0332  | 0.0427  | 0.0534  | 0.0652  | 0.0780  | 0.0920  | 0.1071  | 0.1232  | 0.1405  | 0.1588  |
| 200  | 0.1782  | 0.1987  | 0.2202  | 0.2428  | 0.2665  | 0.2912  | 0.3170  | 0.3438  | 0.3717  | 0.4006  |
| 300  | 0.4305  | 0.4615  | 0.4935  | 0.5266  | 0.5607  | 0.5958  | 0.6319  | 0.6690  | 0.7071  | 0.7462  |
| 400  | 0.7864  | 0.8275  | 0.8696  | 0.9127  | 0.9567  | 1.0018  | 1.0478  | 1.0948  | 1.1427  | 1.1916  |
| 500  | 1.2415  | 1.2923  | 1.3440  | 1.3967  | 1.4503  | 1.5048  | 1.5603  | 1.6166  | 1.6739  | 1.7321  |
| 600  | 1.7912  | 1.8512  | 1.9120  | 1.9738  | 2.0365  | 2.1000  | 2.1644  | 2.2296  | 2.2957  | 2.3627  |
| 700  | 2.4305  | 2.4991  | 2.5686  | 2.6390  | 2.7101  | 2.7821  | 2.8548  | 2.9284  | 3.0028  | 3.0780  |
| 800  | 3.1540  | 3.2308  | 3.3084  | 3.3867  | 3.4658  | 3.5457  | 3.6264  | 3.7078  | 3.7899  | 3.8729  |
| 900  | 3.9565  | 4.0409  | 4.1260  | 4.2119  | 4.2984  | 4.3857  | 4.4737  | 4.5624  | 4.6518  | 4.7419  |
| 1000 | 4.8326  | 4.9241  | 5.0162  | 5.1090  | 5.2025  | 5.2966  | 5.3914  | 5.4868  | 5.5829  | 5.6796  |
| 1100 | 5.7769  | 5.8749  | 5.9734  | 6.0726  | 6.1724  | 6.2728  | 6.3737  | 6.4753  | 6.5774  | 6.6801  |
| 1200 | 6.7833  | 6.8871  | 6.9914  | 7.0963  | 7.2017  | 7.3076  | 7.4140  | 7.5210  | 7.6284  | 7.7363  |
| 1300 | 7.8446  | 7.9534  | 8.0627  | 8.1724  | 8.2826  | 8.3932  | 8.5041  | 8.6155  | 8.7273  | 8.8394  |
| 1400 | 8.9519  | 9.0648  | 9.1780  | 9.2915  | 9.4053  | 9.5194  | 9.6338  | 9.7485  | 9.8634  | 9.9786  |
| 1500 | 10.0940 | 10.2097 | 10.3255 | 10.4415 | 10.5577 | 10.6740 | 10.7905 | 10.9071 | 11.0237 | 11.1405 |
| 1600 | 11.2574 | 11.3743 | 11.4913 | 11.6082 | 11.7252 | 11.8422 | 11.9591 | 12.0761 | 12.1929 | 12.3100 |
| 1700 | 12.4263 | 12.5429 | 12.6594 | 12.7757 | 12.8918 | 13.0078 | 13.1236 | 13.2391 | 13.3545 | 13.4696 |
| 1800 | 13.5845 | 13.6991 | 13.8135 |         |         |         |         |         |         |         |

**TABLE 11.57** Type E Thermocouples: Nickel-Chromium Alloy vs. Copper-Nickel Alloy

*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C   | 0      | 10     | 20     | 30     | 40     | 50     | 60     | 70     | 80     | 90     |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| −200 | −8.824 | −9.063 | −9.274 | −9.455 | −9.604 | −9.719 | −9.797 | −9.835 |        |        |
| −100 | −5.237 | −5.680 | −6.107 | −6.516 | −6.907 | −7.279 | −7.631 | −7.963 | −8.273 | −8.561 |
| −0   | 0.000  | −0.581 | −1.151 | −1.709 | −2.254 | −2.787 | −3.306 | −3.811 | −4.301 | −4.777 |
| 0    | 0.000  | 0.591  | 1.192  | 1.801  | 2.419  | 3.047  | 3.683  | 4.394  | 4.983  | 5.646  |
| 100  | 6.317  | 6.996  | 7.683  | 8.377  | 9.078  | 9.787  | 10.501 | 11.222 | 11.949 | 12.681 |
| 200  | 13.419 | 14.161 | 14.909 | 15.661 | 16.417 | 17.178 | 17.942 | 18.710 | 19.481 | 20.256 |
| 300  | 21.033 | 21.814 | 22.597 | 23.383 | 24.171 | 24.961 | 25.754 | 26.549 | 27.345 | 28.143 |
| 400  | 28.943 | 29.744 | 30.546 | 31.350 | 32.155 | 32.960 | 33.767 | 34.574 | 35.382 | 36.190 |
| 500  | 36.999 | 37.808 | 38.617 | 39.426 | 40.236 | 41.045 | 41.853 | 42.662 | 43.470 | 44.278 |
| 600  | 45.085 | 45.891 | 46.697 | 47.502 | 48.306 | 49.109 | 49.911 | 50.713 | 51.513 | 52.312 |
| 700  | 53.110 | 53.907 | 54.703 | 55.498 | 56.291 | 57.083 | 57.873 | 58.663 | 59.451 | 60.237 |
| 800  | 61.022 | 61.806 | 62.588 | 63.368 | 64.147 | 64.924 | 65.700 | 66.473 | 67.245 | 68.015 |
| 900  | 68.783 | 69.549 | 70.313 | 71.075 | 71.835 | 72.593 | 73.350 | 74.104 | 74.857 | 75.608 |
| 1000 | 76.358 |        |        |        |        |        |        |        |        |        |

**TABLE 11.58** Type J Thermocouples: Iron vs. Copper-Nickel Alloy  
*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C   | 0      | 10     | 20     | 30     | 40     | 50     | 60     | 70     | 80     | 90     |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| −200 | −7.890 | −8.096 |        |        |        |        |        |        |        |        |
| −100 | −4.632 | −5.036 | −5.426 | −5.801 | −6.159 | −6.499 | −6.821 | −7.122 | −7.402 | −7.659 |
| −0   | 0.000  | −0.501 | −0.995 | −1.481 | −1.960 | −2.431 | −2.892 | −3.344 | −3.785 | −4.215 |
| 0    | 0.000  | 0.507  | 1.019  | 1.536  | 2.058  | 2.585  | 3.115  | 3.649  | 4.186  | 4.725  |
| 100  | 5.268  | 5.812  | 6.359  | 6.907  | 7.457  | 8.008  | 8.560  | 9.113  | 9.667  | 10.222 |
| 200  | 10.777 | 11.332 | 11.887 | 12.442 | 12.998 | 13.553 | 14.108 | 14.663 | 15.217 | 15.771 |
| 300  | 16.325 | 16.879 | 17.432 | 17.984 | 18.537 | 19.089 | 19.640 | 20.192 | 20.743 | 21.295 |
| 400  | 21.846 | 22.397 | 22.949 | 23.501 | 24.054 | 24.607 | 25.161 | 25.716 | 26.272 | 26.829 |
| 500  | 27.388 | 27.949 | 28.511 | 29.075 | 29.642 | 30.210 | 30.782 | 31.356 | 31.933 | 32.513 |
| 600  | 33.096 | 33.683 | 34.273 | 34.867 | 35.464 | 36.066 | 36.671 | 37.280 | 37.893 | 38.510 |
| 700  | 39.130 | 39.754 | 40.482 | 41.013 | 41.647 | 42.283 | 42.922 |        |        |        |

**TABLE 11.59** Type K Thermocouples: Nickel-Chromium Alloy vs. Nickel-Aluminum Alloy

*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C   | 0      | 10     | 20     | 30     | 40     | 50     | 60     | 70     | 80     | 90     |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| −200 | −5.891 | −6.035 | −6.158 | −6.262 | −6.344 | −6.404 | −6.441 | −6.458 |        |        |
| −100 | −3.553 | −3.852 | −4.138 | −4.410 | −4.669 | −4.912 | −5.141 | −5.354 | −5.550 | −5.730 |
| −0   | 0.000  | −0.392 | −0.777 | −1.156 | −1.517 | −1.889 | −2.243 | −2.586 | −2.920 | −3.242 |
| 0    | 0.000  | 0.397  | 0.798  | 1.203  | 1.611  | 2.022  | 2.436  | 2.850  | 3.266  | 3.681  |
| 100  | 4.095  | 4.508  | 4.919  | 5.327  | 5.733  | 6.137  | 6.539  | 6.939  | 7.338  | 7.737  |
| 200  | 8.137  | 8.537  | 8.938  | 9.341  | 9.745  | 10.151 | 10.560 | 10.969 | 11.381 | 11.793 |
| 300  | 12.207 | 12.623 | 13.039 | 13.456 | 13.874 | 14.292 | 14.712 | 15.132 | 15.552 | 15.974 |
| 400  | 16.395 | 16.818 | 17.241 | 17.664 | 18.088 | 18.513 | 18.839 | 19.363 | 19.788 | 20.214 |
| 500  | 20.640 | 21.066 | 21.493 | 21.919 | 22.346 | 22.772 | 23.198 | 23.624 | 24.050 | 24.476 |
| 600  | 24.902 | 25.327 | 25.751 | 26.176 | 26.599 | 27.022 | 27.445 | 27.867 | 28.288 | 28.709 |
| 700  | 29.128 | 29.547 | 29.965 | 30.383 | 30.799 | 31.214 | 31.629 | 32.042 | 32.455 | 32.866 |
| 800  | 33.277 | 33.686 | 34.095 | 34.502 | 34.909 | 35.314 | 35.718 | 36.121 | 36.524 | 36.925 |
| 900  | 37.325 | 37.724 | 38.122 | 38.519 | 38.915 | 39.310 | 39.703 | 40.096 | 40.488 | 40.879 |
| 1000 | 41.269 | 41.657 | 42.045 | 42.432 | 42.817 | 43.202 | 43.585 | 43.968 | 44.349 | 44.729 |
| 1100 | 45.108 | 45.486 | 45.863 | 46.238 | 46.612 | 46.985 | 47.356 | 47.726 | 48.095 | 48.462 |
| 1200 | 48.828 | 49.129 | 49.555 | 49.916 | 50.276 | 50.633 | 50.990 | 51.344 | 51.697 | 52.049 |
| 1300 | 52.398 | 52.747 | 53.093 | 53.439 | 53.782 | 54.125 | 54.466 | 54.807 |        |        |

**TABLE 11.60** Type N Thermocouples: Nickel–14.2% Chromium–1.4% Silicon Alloy vs. Nickel–4.4% Silicon–0.1% Magnesium Alloy

*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C   | 0      | 10     | 20     | 30     | 40     | 50     | 60     | 70     | 80     | 90     |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| –200 | –3.990 | –4.083 | –4.162 | –4.227 | –4.277 | –4.313 | –4.336 | –4.345 |        |        |
| –100 | –2.407 | –2.612 | –2.807 | –2.994 | –3.170 | –3.336 | –3.491 | –3.634 | –3.766 | –3.884 |
| –0   | 0.000  | –0.260 | –0.518 | –0.772 | –1.023 | –1.268 | –1.509 | –1.744 | –1.972 | –2.193 |
| 0    | 0.000  | 0.261  | 0.525  | 0.793  | 1.064  | 1.339  | 1.619  | 1.902  | 2.188  | 2.479  |
| 100  | 2.774  | 3.072  | 3.374  | 3.679  | 3.988  | 4.301  | 4.617  | 4.936  | 5.258  | 5.584  |
| 200  | 5.912  | 6.243  | 6.577  | 6.914  | 7.254  | 7.596  | 7.940  | 8.287  | 8.636  | 8.987  |
| 300  | 9.340  | 9.695  | 10.053 | 10.412 | 10.772 | 11.135 | 11.499 | 11.865 | 12.233 | 12.602 |
| 400  | 12.972 | 13.344 | 13.717 | 14.091 | 14.467 | 14.844 | 15.222 | 15.601 | 15.981 | 16.362 |
| 500  | 16.744 | 17.127 | 17.511 | 17.896 | 18.282 | 18.668 | 19.055 | 19.443 | 19.831 | 20.220 |
| 600  | 20.609 | 20.999 | 21.390 | 21.781 | 22.172 | 22.564 | 22.956 | 23.348 | 23.740 | 24.133 |
| 700  | 24.526 | 24.919 | 25.312 | 25.705 | 26.098 | 26.491 | 26.885 | 27.278 | 27.671 | 28.063 |
| 800  | 28.456 | 28.849 | 29.241 | 29.633 | 30.025 | 30.417 | 30.808 | 31.199 | 31.590 | 31.980 |
| 900  | 32.370 | 32.760 | 33.149 | 33.538 | 33.926 | 34.315 | 34.702 | 35.089 | 35.476 | 35.862 |
| 1000 | 36.248 | 36.633 | 37.018 | 37.402 | 37.786 | 38.169 | 38.552 | 38.934 | 39.315 | 39.696 |
| 1100 | 40.076 | 40.456 | 40.835 | 41.213 | 41.590 | 41.966 | 42.342 | 42.717 | 43.091 | 43.464 |
| 1200 | 43.836 | 44.207 | 44.577 | 44.947 | 45.315 | 45.682 | 46.048 | 46.413 | 46.777 | 47.140 |
| 1300 | 47.502 |        |        |        |        |        |        |        |        |        |

**TABLE 11.61** Type R Thermocouples: Platinum–13% Rhodium Alloy vs. Platinum  
*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C           | 0       | 10      | 20      | 30      | 40      | 50      | 60      | 70      | 80      | 90      |
|--------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| (Below zero) |         | −0.0515 | −0.100  | −0.1455 | −0.1877 | −0.2264 |         |         |         |         |
| 0            | 0.0000  | 0.0543  | 0.1112  | 0.1706  | 0.2324  | 0.2965  | 0.3627  | 0.4310  | 0.5012  | 0.5733  |
| 100          | 0.6472  | 0.7228  | 0.8000  | 0.8788  | 0.9591  | 1.0407  | 1.1237  | 1.2080  | 1.2936  | 1.3803  |
| 200          | 1.4681  | 1.5571  | 1.6471  | 1.7381  | 1.8300  | 1.9229  | 2.0167  | 2.1113  | 2.2068  | 2.3030  |
| 300          | 2.4000  | 2.4978  | 2.5963  | 2.6954  | 2.7953  | 2.8957  | 2.9968  | 3.0985  | 3.2009  | 3.3037  |
| 400          | 3.4072  | 3.5112  | 3.6157  | 3.7208  | 3.8264  | 3.9325  | 4.0391  | 4.1463  | 4.2539  | 4.3620  |
| 500          | 4.4706  | 4.5796  | 4.6892  | 4.7992  | 4.9097  | 5.0206  | 5.1320  | 5.2439  | 5.3562  | 5.4690  |
| 600          | 5.5823  | 5.6960  | 5.8101  | 5.9246  | 6.0398  | 6.1554  | 6.2716  | 6.3883  | 6.5054  | 6.6230  |
| 700          | 6.7412  | 6.8598  | 6.9789  | 7.0984  | 7.2185  | 7.3390  | 7.4600  | 7.5815  | 7.7035  | 7.8259  |
| 800          | 7.9488  | 8.0722  | 8.1960  | 8.3203  | 8.4451  | 8.5703  | 8.6960  | 8.8222  | 8.9488  | 9.0758  |
| 900          | 9.2034  | 9.3313  | 9.4597  | 9.5886  | 9.7179  | 9.8477  | 9.9779  | 10.1086 | 10.2397 | 10.3712 |
| 1000         | 10.5032 | 10.6356 | 10.7684 | 10.9017 | 11.0354 | 11.1695 | 11.3041 | 11.4391 | 11.5745 | 11.7102 |
| 1100         | 11.8463 | 11.9827 | 12.1194 | 12.2565 | 12.3939 | 12.5315 | 12.6695 | 12.8077 | 12.9462 | 13.0849 |
| 1200         | 13.2239 | 13.3631 | 13.5025 | 13.6421 | 13.7818 | 13.9218 | 14.0619 | 14.2022 | 14.3426 | 14.4832 |
| 1300         | 14.6239 | 14.7647 | 14.9056 | 15.0465 | 15.1876 | 15.3287 | 15.4699 | 15.6110 | 15.7522 | 15.8935 |
| 1400         | 16.0347 | 16.1759 | 16.3172 | 16.4583 | 16.5995 | 16.7405 | 16.8816 | 17.0225 | 17.1634 | 17.3041 |
| 1500         | 17.4447 | 17.5852 | 17.7256 | 17.8659 | 18.0059 | 18.1458 | 18.2855 | 18.4251 | 18.5644 | 18.7035 |
| 1600         | 18.8424 | 18.9810 | 19.1194 | 19.2575 | 19.3953 | 19.5329 | 19.6702 | 19.8071 | 19.9437 | 20.0797 |
| 1700         | 20.2151 | 20.3497 | 20.4834 | 20.6161 | 20.7475 | 20.8777 | 21.0064 |         |         |         |

**TABLE 11.62** Type S Thermocouples: Platinum–10% Rhodium Alloy vs. Platinum  
*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C           | 0       | 10      | 20      | 30      | 40      | 50      | 60      | 70      | 80      | 90      |
|--------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| (Below zero) |         | −0.0527 | −0.1028 | −0.1501 | −0.1944 | −0.2357 |         |         |         |         |
| 0            | 0.0000  | 0.0552  | 0.1128  | 0.1727  | 0.2347  | 0.2986  | 0.3646  | 0.4323  | 0.5017  | 0.5728  |
| 100          | 0.6453  | 0.7194  | 0.7948  | 0.8714  | 0.9495  | 1.0287  | 1.1089  | 1.1902  | 1.2726  | 1.3558  |
| 200          | 1.4400  | 1.5250  | 1.6109  | 1.6975  | 1.7849  | 1.8729  | 1.9617  | 2.0510  | 2.1410  | 2.2316  |
| 300          | 2.3227  | 2.4143  | 2.5065  | 2.5991  | 2.6922  | 2.7858  | 2.8798  | 2.9742  | 3.0690  | 3.1642  |
| 400          | 3.2597  | 3.3557  | 3.4519  | 3.5485  | 3.6455  | 3.7427  | 3.8403  | 3.9382  | 4.0364  | 4.1348  |
| 500          | 4.2336  | 4.3327  | 4.4320  | 4.5316  | 4.6316  | 4.7318  | 4.8323  | 4.9331  | 5.0342  | 5.1356  |
| 600          | 5.2373  | 5.3394  | 5.4417  | 5.5445  | 5.6477  | 5.7513  | 5.8553  | 5.9595  | 6.0641  | 6.1690  |
| 700          | 6.2743  | 6.3799  | 6.4858  | 6.5920  | 6.6986  | 6.8055  | 6.9127  | 7.0202  | 7.1281  | 7.2363  |
| 800          | 7.3449  | 7.4537  | 7.5629  | 7.6724  | 7.7823  | 7.8925  | 8.0030  | 8.1138  | 8.2250  | 8.3365  |
| 900          | 8.4483  | 8.5605  | 8.6730  | 8.7858  | 8.8989  | 9.0124  | 9.1262  | 9.2403  | 9.3548  | 9.4696  |
| 1000         | 9.5847  | 9.7002  | 9.8159  | 9.9320  | 10.0485 | 10.1652 | 10.2823 | 10.3997 | 10.5174 | 10.6354 |
| 1100         | 10.7536 | 10.8720 | 10.9907 | 11.1095 | 11.2286 | 11.3479 | 11.4674 | 11.5871 | 11.7069 | 11.8269 |
| 1200         | 11.9471 | 12.0674 | 12.1878 | 12.3084 | 12.4290 | 12.5498 | 12.6707 | 12.7917 | 12.9127 | 13.0338 |
| 1300         | 13.1550 | 13.2762 | 13.3975 | 13.5188 | 13.6401 | 13.7614 | 13.8828 | 14.0041 | 14.1254 | 14.2467 |
| 1400         | 14.3680 | 14.4892 | 14.6103 | 14.7314 | 14.8524 | 14.9734 | 15.0942 | 15.2150 | 15.3356 | 15.4561 |
| 1500         | 15.5765 | 15.6967 | 15.8168 | 15.9368 | 16.0566 | 16.1762 | 16.2956 | 16.4148 | 16.5338 | 16.6526 |
| 1600         | 16.7712 | 16.8895 | 17.0076 | 17.1255 | 17.2431 | 17.3604 | 17.4474 | 17.5942 | 17.7105 | 17.8264 |
| 1700         | 17.9417 | 18.0562 | 18.1698 | 18.2823 | 18.3937 | 18.5038 | 18.6124 |         |         |         |

**TABLE 11.63** Type T Thermocouples: Copper vs. Copper-Nickel Alloy  
*Thermoelectric voltage in millivolts; reference junction at 0°C.*

| °C   | 0      | 10     | 20     | 30     | 40     | 50     | 60     | 70     | 80     | 90     |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| −200 | −5.603 | −5.753 | −5.889 | −6.007 | −6.105 | −6.181 | −6.232 | −6.258 |        |        |
| −100 | −3.378 | −3.656 | −3.923 | −4.177 | −4.419 | −4.648 | −4.865 | −5.069 | −5.261 | −5.439 |
| −0   | 0.000  | −0.383 | −0.757 | −1.121 | −1.475 | −1.819 | −2.152 | −2.475 | −2.788 | −3.089 |
| 0    | 0.000  | 0.391  | 0.789  | 1.196  | 1.611  | 2.035  | 2.467  | 2.908  | 3.357  | 3.813  |
| 100  | 4.277  | 4.749  | 5.227  | 5.712  | 6.204  | 6.702  | 7.207  | 7.718  | 8.235  | 8.757  |
| 200  | 9.286  | 9.820  | 10.360 | 10.905 | 11.456 | 12.011 | 12.572 | 13.137 | 13.707 | 14.281 |
| 300  | 14.860 | 15.443 | 16.030 | 16.621 | 17.217 | 17.816 | 18.420 | 19.027 | 19.638 | 20.252 |
| 400  | 20.869 |        |        |        |        |        |        |        |        |        |



11.11 CORRECTION FOR EMERGENT STEM OF THERMOMETERS

When a thermometer which has been standardized for total immersion is used with a part of the liquid column at a temperature below that of the bulb, the reading is low and a correction must be applied. The stem correction, in degrees Celsius, is given by

$KL(t_o - t_m) = \text{degrees Celsius}$

- where  $K$  = constant, characteristic of the particular kind of glass and temperature (see Table 11.49)
- $L$  = length of exposed thermometer, °C (that is, the length not in contact with vapor or liquid being measured)
- $t_o$  = observed temperature on thermometer
- $t_m$  = mean temperature of exposed column (obtained by placing an auxiliary thermometer alongside with its bulb midpoint)

For thermometers containing organic liquids, it is sufficient to use the approximate value,  $K = 0.001$ . In such thermometers the value of  $K$  is practically independent of the kind of glass.

TABLE 11.64 Values of  $K$  for Stem Correction of Thermometers

| Temperature, °C | Soft glass | Heat-resistant glass |
|-----------------|------------|----------------------|
| 0–150           | 0.000 158  | 0.000 165            |
| 200             | 0.000 159  | 0.000 167            |
| 250             | 0.000 161  | 0.000 170            |
| 300             | 0.000 164  | 0.000 174            |
| 350             |            | 0.000 178            |
| 400             |            | 0.000 183            |
| 450             |            | 0.000 188            |

**Index Terms****Links**

## Abbreviations:

|                                       |        |
|---------------------------------------|--------|
| of amino acids, 3 letter and 1 letter | 11.102 |
| of ligand names                       | 3.11   |
| mathematical                          | 2.23   |
| of SI units                           | 2.3    |
| of states of aggregation              | 2.6    |
| of words                              | 2.26   |

|                |       |
|----------------|-------|
| ABS copolymers | 10.20 |
| properties of  | 10.50 |

|                        |      |
|------------------------|------|
| Absolute configuration | 1.49 |
|------------------------|------|

## Absorbance:

|                              |      |
|------------------------------|------|
| defined                      | 7.39 |
| to percent absorption, table | 2.96 |
| to transmittance, table      | 2.98 |

|                                                   |      |
|---------------------------------------------------|------|
| Absorption bands, electronic, for<br>chromophores | 7.19 |
|---------------------------------------------------|------|

|                                      |      |
|--------------------------------------|------|
| Absorption cross section of nuclides | 4.58 |
|--------------------------------------|------|

|                                         |     |
|-----------------------------------------|-----|
| Absorption edges, X-ray, wavelengths of | 7.8 |
|-----------------------------------------|-----|

|                       |       |
|-----------------------|-------|
| Absorption indicators | 11.95 |
|-----------------------|-------|

|                                      |     |
|--------------------------------------|-----|
| Absorption energies, X-ray, critical | 7.7 |
|--------------------------------------|-----|

|                                       |      |
|---------------------------------------|------|
| Absorption lines, atomic, of elements | 7.29 |
|---------------------------------------|------|

|                                                            |       |
|------------------------------------------------------------|-------|
| Absorption maxima, wavelengths, of<br>acid-base indicators | 8.116 |
|------------------------------------------------------------|-------|

|                                                         |      |
|---------------------------------------------------------|------|
| Absorption, percent, conversion to<br>absorbance, table | 2.96 |
|---------------------------------------------------------|------|

|                       |      |
|-----------------------|------|
| Absorptivity, defined | 7.38 |
|-----------------------|------|

## Abundance, natural:

|             |           |
|-------------|-----------|
| of isotopes | 4.81      |
| of nuclides | 4.59 7.89 |

|          |       |
|----------|-------|
| Accuracy | 2.118 |
|----------|-------|

|                   |            |
|-------------------|------------|
| Acetal copolymers | 10.8 10.22 |
|-------------------|------------|

|                     |            |
|---------------------|------------|
| Acetal homopolymers | 10.8 10.22 |
|---------------------|------------|

|                                |       |
|--------------------------------|-------|
| Acetal polymers, properties of | 10.22 |
|--------------------------------|-------|

## Acetals:

|                                                     |            |
|-----------------------------------------------------|------------|
| nomenclature of                                     | 1.23       |
| as plastic materials, formulas and<br>properties of | 10.8 10.22 |

|                                   |      |
|-----------------------------------|------|
| Acetamide, binary azeotropes with | 5.74 |
|-----------------------------------|------|

|                                   |      |
|-----------------------------------|------|
| Acetate, formation constants with | 8.88 |
|-----------------------------------|------|

## Acetic acid:

|                         |      |
|-------------------------|------|
| binary azeotropes with  | 5.63 |
| pKa values of           | 8.81 |
| ternary azeotropes with | 5.80 |

|                                 |      |
|---------------------------------|------|
| Acetone, binary azeotropes with | 5.74 |
| pKa values in                   | 8.81 |

## Acetonitrile:

|                          |      |
|--------------------------|------|
| formation constants with | 8.88 |
| pKa values in            | 8.81 |

|                                         |      |
|-----------------------------------------|------|
| Acetylacetone, formation constants with | 8.88 |
|-----------------------------------------|------|

|                                                           |     |
|-----------------------------------------------------------|-----|
| Acetylene, solubility in water at various<br>temperatures | 5.3 |
|-----------------------------------------------------------|-----|

## Acid anhydrides:

|                         |      |
|-------------------------|------|
| infrared frequencies of | 7.50 |
| nomenclature of         | 1.23 |
| Raman frequencies of    | 7.78 |

**Index Terms****Links**

|                                         |        |       |
|-----------------------------------------|--------|-------|
| Acid-base indicators                    | 8.115  |       |
| Acid-base titrations:                   |        |       |
| indicators for                          | 8.116  |       |
| primary standards for                   | 11.74  |       |
| volumetric (titrimetric) factors for    | 11.76  |       |
| Acid chlorides, infrared frequencies of | 7.50   |       |
| Acid dissociation constants:            |        |       |
| Harnmett and Taft equations for         |        |       |
| estimation of                           | 9.2    |       |
| of indicators                           | 8.116  |       |
| of inorganic materials                  | 8.18   |       |
| of organic materials                    | 8.24   |       |
| at various temperatures                 | 8.73   |       |
| Acid halides:                           |        |       |
| infrared frequencies of                 | 7.50   |       |
| Raman frequencies of                    | 7.78   |       |
| Acid halogenides                        | 3.8    |       |
| Acid peroxides, infrared frequencies of | 7.50   |       |
| Acid titrants, volumetric factors for   | 11.76  |       |
| Acid value:                             |        |       |
| of fats and oils                        | 10.69  |       |
| of waxes                                | 10.72  |       |
| Acids:                                  |        |       |
| concentrations of commonly used         | 11.106 |       |
| functional derivatives of inorganic,    |        |       |
| nomenclature of                         | 3.8    |       |
| inorganic, nomenclature of              | 3.8    |       |
| organic, nomenclature of                | 1.29   | 1.38  |
| standardization of basic solutions      | 11.75  |       |
| trivial names for inorganic (table)     | 3.8    |       |
| Acrylic poly(vinyl chloride) alloy,     |        |       |
| properties of                           | 10.24  |       |
| Acrylic polymers:                       |        |       |
| description of                          | 10.8   |       |
| properties of                           | 10.8   | 10.24 |
| Acrylonitrile-butadiene-styrene (ABS)   |        |       |
| copolymers                              | 10.19  |       |
| Acrylonitrile- butadiene-styrene-poly   |        |       |
| ( vinyl chloride ) alloy, properties of | 10.24  |       |
| Activity coefficients                   | 8.2    |       |
| at high ionic strengths                 | 8.5    |       |
| Acyclic conformation isomers            | 1.39   |       |
| Acyl halides, nomenclature of           | 1.24   |       |
| Acylals, nomenclature of                | 1.23   |       |
| Addition compounds, nomenclature of     | 3.112  |       |
| Additives to polymers                   | 10.4   |       |
| Adjusted retention time                 | 11.27  |       |
| Adsorption indicators                   | 11.95  |       |
| Affinities, electron:                   |        |       |
| of atoms                                | 4.24   |       |
| of molecules                            | 4.25   |       |
| of radicals                             | 4.27   |       |
| Affixes, multiplying                    | 1.21   |       |

| <b><u>Index Terms</u></b>                                                | <b><u>Links</u></b> |       |
|--------------------------------------------------------------------------|---------------------|-------|
| Aggregation, states of, abbreviations for                                | 2.7                 |       |
| Air:                                                                     |                     |       |
| autoignition temperatures of combustible mixtures                        | 5.139               |       |
| buoyancy reduction factor for weighings                                  | 2.83                |       |
| flammable limits of combustible mixtures in                              | 5.139               |       |
| moist, density of                                                        | 5.88                |       |
| refractive index of                                                      | 5.135               |       |
| saturated, mass of water vapor in at various temperatures                | 5.156               |       |
| solubility in water at various temperatures                              | 5.3                 |       |
| specific gravity at various temperatures                                 | 5.88                |       |
| Alcoholometer                                                            | 2.66                |       |
| Alcohols:                                                                |                     |       |
| binary azeotropes with                                                   | 5.57                | 5.66  |
| nomenclature of                                                          | 1.24                |       |
| retained trivial names of                                                | 1.24                |       |
| ternary azeotropes with                                                  | 5.81                |       |
| Aldehydes:                                                               |                     |       |
| binary azeotropes with                                                   | 5.59                |       |
| infrared frequencies of                                                  | 7.51                |       |
| nomenclature of                                                          | 1.26                |       |
| Raman frequencies of                                                     | 7.78                |       |
| Alicyclic ring systems, carbon-13 chemical shifts                        | 7.101               |       |
| Aliphatic hydrocarbons, monocyclic, nomenclature of                      | 1.5                 |       |
| Alizarin red, formation constants with                                   | 8.89                |       |
| Alkali titrants, volumetric factors for                                  | 11.77               |       |
| Alkane carbon-hydrogen and carbon-carbon bonds                           |                     |       |
| Raman frequencies of                                                     | 7.71                |       |
| Alkane carbons, estimation of carbon-13 chemical shifts                  | 7.102               |       |
| Alkane residues, infrared frequencies of                                 | 7.41                |       |
| Alkanes:                                                                 |                     |       |
| carbon-13 chemical shifts                                                | 7.102               |       |
| nomenclature of                                                          | 1.1                 |       |
| proton chemical shifts                                                   | 7.92                |       |
| Raman frequencies of                                                     | 7.71                |       |
| Alkenes:                                                                 |                     |       |
| carbon-13 chemical shifts                                                | 7.103               |       |
| infrared frequencies of                                                  | 7.54                |       |
| nomenclature of                                                          | 1.4                 |       |
| proton chemical shifts                                                   | 7.92                |       |
| Raman frequencies of                                                     | 7.79                |       |
| Alkyd molding polymers, properties of                                    | 10.24               | 10.42 |
| Alkyd polyester thermosetting polymers, properties of                    | 10.42               |       |
| Alkyd polymers                                                           | 10.9                |       |
| Alkyl carbon-13 chemical shifts, effect of substituents upon             | 7.102               |       |
| Alkyl groups, effects of substituent groups on carbon-13 chemical shifts | 7.102               |       |

| <b><u>Index Terms</u></b>                   | <b><u>Links</u></b> |       |
|---------------------------------------------|---------------------|-------|
| Alkynes, nomenclature of                    | 1.4                 |       |
| Allotropes                                  | 3.5                 |       |
| Alloy polymers:                             |                     |       |
| description of                              | 10.10               |       |
| properties of                               | 10.24               |       |
| Allyl alcohol:                              |                     |       |
| binary azeotropes with                      | 5.71                |       |
| ternary azeotropes with                     | 5.78                |       |
| Allyl polymers:                             |                     |       |
| description of                              | 10.10               |       |
| properties of                               | 10.26               |       |
| Allyl-diglycol-carbonate polymer,           |                     |       |
| properties of                               | 10.26               |       |
| Alphabet, Greek                             | 2.25                |       |
| Alternate names of organic compounds        | 1.74                | 1.76  |
| Alternative hypothesis                      | 2.126               |       |
| Altitude-gravity correction in barometry    | 2.77                |       |
| Altitude-temperature factor in barometry    | 2.78                |       |
| Alumina, solvent strength parameters        | 11.16               |       |
| Aluminum:                                   |                     |       |
| bond dissociation energies                  | 4.41                |       |
| gravimetric factors                         | 11.41               |       |
| Amides:                                     |                     |       |
| infrared frequencies of                     | 7.52                |       |
| inorganic                                   | 3.9                 |       |
| nomenclature of                             | 1.27                |       |
| Amidines, infrared frequencies of           | 7.54                |       |
| Amines:                                     |                     |       |
| binary azeotropes with                      | 5.59                |       |
| infrared frequencies of                     | 7.41                |       |
| nomenclature of                             | 1.27                |       |
| Amino acids, pI and pKa values              | 11.102              |       |
| Ammonia:                                    |                     |       |
| formation constants with                    | 8.83                |       |
| liquid, vapor pressure of                   | 5.27                |       |
| solubility in water at various temperatures | 5.3                 |       |
| Ammoniameter                                | 2.66                |       |
| Ammonium compounds:                         |                     |       |
| gravimetric factors                         | 11.41               |       |
| nomenclature of                             | 1.28                |       |
| Ammonium ion, infrared frequencies of       | 7.46                |       |
| Amorphous polymers                          | 10.2                |       |
| Amount of substance                         | 2.3                 |       |
| Ampere, definition of                       | 2.3                 |       |
| Analytical reagents for gravimetry          | 11.67               |       |
| Analytical weights, tolerances for          | 11.71               |       |
| Analyzing crystals, for X-ray spectroscopy  | 7.13                |       |
| Angle, trigonometric functions of           | 2.113               | 2.115 |
| Angles in unit cells                        | 4.58                |       |
| Anhydrides, of inorganic acids              | 3.9                 |       |
| Aniline, binary azeotropes with             | 5.75                |       |
| Animal fats and oils, properties of         | 10.69               |       |
| Anion-exchange resins, guide to (table)     | 11.33               |       |

| <b><u>Index Terms</u></b>                                    | <b><u>Links</u></b> |       |
|--------------------------------------------------------------|---------------------|-------|
| Anions, inorganic:                                           |                     |       |
| nomenclature of                                              | 3.6                 | 3.10  |
| selectivity coefficients in ion exchange                     | 11.38               |       |
| Anomalous electron moment correction                         | 2.4                 |       |
| Antifreeze solutions, aqueous                                | 5.83                |       |
| Antimony:                                                    |                     |       |
| bond dissociation energies                                   | 4.41                |       |
| gravimetric factors                                          | 11.42               |       |
| Antioxidants for polymers                                    | 10.4                |       |
| Antistatic agents for polymers                               | 10.4                |       |
| Antoine equation                                             | 5.29                |       |
| Aqueous tension of solutions                                 | 11.6                |       |
| Aramid polymer, properties of                                | 10.38               |       |
| Areas:                                                       |                     |       |
| between abscissa values of normal<br>distribution curve      | 2.122               |       |
| by approximation                                             | 2.111               |       |
| of surfaces                                                  | 2.109               |       |
| Argon, solubility in water at various<br>temperatures        | 5.8                 |       |
| Argon ICP, detection limits of elements<br>(table)           | 7.29                |       |
| Argon-ion laser plasma lines                                 | 7.88                |       |
| Arithmetic means of set of numbers                           | 2.118               |       |
| Arithmetic mean                                              | 2.118               |       |
| Aromatic bands, infrared frequencies of                      | 7.57                |       |
| Aromatic compounds:                                          |                     |       |
| carbon-13 chemical shifts                                    | 7.104               | 7.105 |
| monocyclic, nomenclature of                                  | 1.5                 |       |
| proton chemical shifts                                       | 7.96                |       |
| Raman frequencies of                                         | 7.82                |       |
| Aromatic nylon polymer, properties of                        | 10.38               |       |
| Aromatic polyester polymers, properties of                   | 10.42               |       |
| Arsenazo, formation constants with                           | 8.89                |       |
| Arsenic:                                                     |                     |       |
| bond dissociation energies                                   | 4.41                |       |
| gravimetric factors                                          | 11.43               |       |
| Astatine bond dissociation energy                            | 4.41                |       |
| Atmospheres, conversion to other<br>pressure units           | 2.87                |       |
| Atom radius of an element                                    | 4.29                |       |
| Atomic absorption:                                           |                     |       |
| electrothermal, detection limits of<br>elements to           | 7.29                |       |
| flame, detection limits of elements                          | 7.29                |       |
| Atomic and group refractions (table)                         | 5.136               |       |
| Atomic fluorescence, plasma, detection<br>limits of elements | 7.29                |       |
| Atomic mass constant                                         | 2.4                 |       |
| Atomic number of elements                                    | 4.2                 |       |
| Atomic quantities, symbols, SI units and<br>definitions      | 2.6                 |       |
| Atomic refractions                                           | 5.135               |       |
| Atoms, electron affinities of                                | 4.24                |       |

| <b><u>Index Terms</u></b>                               | <b><u>Links</u></b> |       |
|---------------------------------------------------------|---------------------|-------|
| Aurintricarboxylic acid, formation constants with       | 8.89                |       |
| Autoignition temperature of combustible mixtures in air | 5.139               |       |
| Average linear velocity of mobile phase                 | 11.27               |       |
| Avogadro number constant                                | 2.4                 | 5.169 |
| Axes in unit cells                                      | 4.58                |       |
| Azeotropic mixtures:                                    |                     |       |
| binary                                                  | 5.58                |       |
| ternary                                                 | 5.77                |       |
| Azo compounds:                                          |                     |       |
| infrared frequencies of                                 | 7.55                |       |
| nomenclature of                                         | 1.28                |       |
| Raman frequencies of                                    | 7.81                |       |
| Azoxy compounds:                                        |                     |       |
| infrared frequencies of                                 | 7.55                |       |
| nomenclature of                                         | 1.28                |       |
| Balling hydrometer                                      | 2.68                |       |
| Band asymmetry                                          | 11.28               |       |
| Barium:                                                 |                     |       |
| bond dissociation energies                              | 4.41                |       |
| gravimetric factors                                     | 11.43               |       |
| Barkometer (barkrometer)                                | 2.66                |       |
| Barometric corrections:                                 |                     |       |
| for capillarity                                         | 2.71                | 2.75  |
| for latitude-gravity                                    | 2.75                |       |
| reduction to sea level                                  | 2.78                |       |
| for temperature                                         | 2.72                |       |
| Barometry                                               | 2.7                 |       |
| Base width of chromatographic peak                      | 11.29               |       |
| Bases:                                                  |                     |       |
| concentration of commonly used                          | 11.106              |       |
| primary standards for aqueous acidic solutions          | 11.74               |       |
| Bates brewers' saccharometer                            | 2.68                |       |
| Bates-Guggenheim convention for pH                      | 8.115               |       |
| Baume degrees, conversion to density                    | 2.85                |       |
| Baume hydrometers                                       | 2.67                |       |
| Beck's hydrometer                                       | 2.67                |       |
| Beer's law                                              | 7.39                |       |
| Beilstein's Handbuch references for organic compounds   | 1.74                | 1.76  |
| Benzene:                                                |                     |       |
| absorption bands (ultraviolet) of                       | 7.23                |       |
| binary azeotropes with                                  | 5.76                |       |
| carbon-13 chemical shifts in substituted                | 7.104               |       |
| proton chemical shifts in monosubstituted               | 7.96                |       |
| Raman frequencies of substitution patterns              | 7.82                |       |
| vapor permeability of polymers                          | 10.69               |       |
| Benzene ring, substitution patterns, Raman frequencies  | 7.83                |       |

| <u>Index Terms</u>                                           | <u>Links</u> |
|--------------------------------------------------------------|--------------|
| Benzoylacetone, formation constants with                     | 8.89         |
| Benzyl alcohol, binary azeotropic mixtures                   | 5.71         |
| Berthelot's equation of state                                | 5.170        |
| Beryllium:                                                   |              |
| bond dissociation energies                                   | 4.41         |
| gravimetric factors                                          | 11.44        |
| Best-fit line                                                | 2.133        |
| errors in slope and intercept                                | 2.135        |
| Binary azeotropes                                            | 5.58         |
| containing alcohols                                          | 5.66         |
| containing ketones                                           | 5.74         |
| containing organic acids                                     | 5.62         |
| containing water                                             | 5.58         |
| Binary compounds between nonmetals                           | 3.2          |
| Biological buffers, pH range                                 | 8.110        |
| Biological materials, pH measurement of                      | 8.106        |
| Bis(2-hydroxyethyl) ether, binary azeotropes with            | 5.76         |
| Bismuth:                                                     |              |
| bond dissociation energies                                   | 4.42         |
| gravimetric factors                                          | 11.44        |
| Bisphenol epoxy resin, properties of                         | 10.28        |
| Bivalent sulfur, nomenclature of                             | 1.37         |
| Blackbody radiation                                          | 7.38    7.39 |
| Blaze wavelength                                             | 7.40         |
| Block copolymers                                             | 10.3         |
| of styrene, properties of                                    | 10.54        |
| Blood, pH measurement of                                     | 8.106        |
| Body-centered cubic structure                                | 4.57         |
| Bohr magneton                                                | 2.4          |
| Bohr radius                                                  | 2.4          |
| Boiling point:                                               |              |
| of chromatographic solvents                                  | 11.16        |
| of inorganic compounds                                       | 3.14         |
| molecular elevation of                                       | 11.13        |
| of organic compounds                                         | 1.76         |
| organic solvents arranged by                                 | 11.10        |
| of water at various pressures                                | 5.56         |
| Boiling point temperature, calculation of                    | 5.30         |
| Boltzmann constant                                           | 2.4          |
| Bond dipole moments                                          | 4.53         |
| Bond dissociation energies                                   | 4.41         |
| Bond lengths and strengths                                   | 4.29         |
| <i>(See also entries for specific elements)</i>              |              |
| Bonds, spatial orientation of                                | 4.56         |
| Borate, reference pH buffer solution at various temperatures | 8.105        |
| Boron:                                                       |              |
| bond dissociation energies                                   | 4.42         |
| bond lengths with other elements                             | 4.39         |
| gravimetric factors                                          | 11.44        |
| Boron compounds:                                             |              |
| infrared frequencies of                                      | 7.61         |
| nomenclature of                                              | 1.29         |



| <u>Index Terms</u>                             | <u>Links</u> |      |
|------------------------------------------------|--------------|------|
| Boron-11 chemical shifts                       | 7.111        |      |
| Boyle's law                                    | 5.169        |      |
| Branched polymers                              | 10.3         |      |
| BR rubber                                      | 10.59        |      |
| Bragg equation                                 | 7.40         |      |
| Bridged hydrocarbons, nomenclature of          | 1.10         |      |
| Briggsian system of logarithms                 | 2.102        |      |
| Brix hydrometer                                | 2.67         | 2.68 |
| Bromide, formation constants with              | 8.84         |      |
| Bromine:                                       |              |      |
| bond dissociation energies                     | 4.42         |      |
| gravimetric factors                            | 11.44        |      |
| overpotential of                               | 8.140        |      |
| solubility in water at various temperatures    | 5.3          |      |
| Buffer solutions:                              |              |      |
| for control purposes                           | 8.110        |      |
| standard reference                             | 8.104        |      |
| Buna N rubber                                  | 10.59        |      |
| Buna S rubber                                  | 10.61        |      |
| Buoyancy effect when weighing in air           | 2.83         |      |
| Burets, tolerances for                         | 11.103       |      |
| Burning rate of polymers                       | 10.22        |      |
| Butadiene-maleic acid copolymer,               |              |      |
| properties of                                  | 10.42        |      |
| 1-Butanol:                                     |              |      |
| binary azeotropes with                         | 5.69         |      |
| ternary azeotropes with                        | 5.78         |      |
| 2-Butanol, ternary azeotropes with             | 5.78         |      |
| 2-Butanone, binary azeotropes with             | 5.74         |      |
| 2-Butoxyethanol, binary azeotropes with        | 5.72         |      |
| Butyl rubber                                   | 10.60        |      |
| Butyric acid, binary azeotropes with           | 5.64         |      |
| Cadmium:                                       |              |      |
| bond dissociation energies                     | 4.42         |      |
| gravimetric factors                            | 11.44        |      |
| Calcium:                                       |              |      |
| bond dissociation energies                     | 4.42         |      |
| gravimetric factors                            | 11.45        |      |
| Calcium chloride solutions, percent            |              |      |
| humidity of                                    | 11.7         |      |
| Calcium hydroxide reference pH buffer          |              |      |
| solution at various temperatures               | 8.105        |      |
| Calibration of conductivity vessels            | 8.160        |      |
| Calmagite, formation constants with            | 8.90         |      |
| Calomel reference electrodes, EMF as           |              |      |
| function of temperature                        | 8.113        |      |
| Candela, definition of                         | 2.3          |      |
| Capacity factor ( <i>see Partition ratio</i> ) |              |      |
| Capillarity correction for barometer           | 2.75         |      |
| Carbon:                                        |              |      |
| attached to double bond, estimation of         |              |      |
| chemical shifts of                             | 7.103        |      |
| bond dissociation energies                     | 4.42         |      |
| gravimetric factors                            | 11.46        |      |

**Index Terms****Links**

|                                                                                                        |       |      |
|--------------------------------------------------------------------------------------------------------|-------|------|
| Carbon-carbon:                                                                                         |       |      |
| bond lengths                                                                                           | 4.36  |      |
| single bonds, Raman frequencies of                                                                     | 7.75  |      |
| spin coupling constants                                                                                | 7.108 |      |
| Carbon dioxide:                                                                                        |       |      |
| gas permeability of polymers and rubbers                                                               | 10.66 |      |
| solubility in water at various temperatures                                                            | 5.4   |      |
| Carbon-fluorine spin coupling constants                                                                | 7.109 |      |
| Carbon-halogen bond lengths                                                                            | 4.36  |      |
| Carbon-hydrogen:                                                                                       |       |      |
| bond lengths                                                                                           | 4.37  |      |
| infrared absorption frequencies                                                                        | 7.41  |      |
| Raman frequencies                                                                                      | 7.71  |      |
| spin coupling constants                                                                                | 7.107 |      |
| Carbon-metals bond lengths                                                                             | 4.38  |      |
| Carbon monoxide solubility in water at<br>various temperatures                                         | 5.4   |      |
| Carbon-nitrogen, bond lengths                                                                          | 4.37  |      |
| Carbon-nitrogen bonds, Raman frequencies of                                                            | 7.74  |      |
| Carbon-nitrogen double bonds, Raman<br>frequencies of                                                  | 7.77  | 7.80 |
| Carbon-nitrogen spin coupling constants                                                                | 7.116 |      |
| Carbon-oxygen bond lengths                                                                             | 4.37  |      |
| Carbon-selenium bond lengths                                                                           | 4.38  |      |
| Carbon-silicon bond lengths                                                                            | 4.38  |      |
| Carbon-sulfur bond lengths                                                                             | 4.38  |      |
| Carbon tetrachloride vapor permeability<br>for polymers                                                | 10.69 |      |
| Carbon-13:                                                                                             |       |      |
| alkanes, estimation of chemical shifts of<br>attached to double bond, estimation of<br>chemical shifts | 7.102 |      |
| chemical shifts                                                                                        | 7.103 |      |
| of carbonyl groups                                                                                     | 7.99  |      |
| in substituted benzenes                                                                                | 7.106 |      |
| in substituted pyridines                                                                               | 7.104 |      |
| Carbon-13 spin coupling constants                                                                      | 7.105 |      |
| Carbon-13 spin coupling constants                                                                      | 7.107 |      |
| Carbonate reference pH buffer solution<br>at various temperatures                                      | 8.105 |      |
| Carbonyl groups:                                                                                       |       |      |
| carbon-13 chemical shifts                                                                              | 7.106 |      |
| infrared frequencies of                                                                                | 7.5   |      |
| Raman frequencies of                                                                                   | 7.78  |      |
| Carboxylate ions, Raman frequencies of                                                                 | 7.79  |      |
| Carboxylic acids:                                                                                      |       |      |
| infrared frequencies of                                                                                | 7.52  |      |
| nomenclature of                                                                                        | 1.29  |      |
| Raman frequencies of                                                                                   | 7.79  |      |
| Carter's hydrometer                                                                                    | 2.67  |      |
| Cations                                                                                                |       |      |
| exchange resins for (guide)                                                                            | 11.34 |      |
| inorganic, nomenclature of                                                                             | 3.6   |      |
| relative selectivity in ion exchange                                                                   | 11.37 |      |

| <b><u>Index Terms</u></b>                 | <b><u>Links</u></b> |
|-------------------------------------------|---------------------|
| Cellulose acetate polymers:               |                     |
| description of                            | 10.10               |
| properties of                             | 10.26               |
| Cellulose-acetate-butyrate polymer:       |                     |
| description of                            | 10.11               |
| properties of                             | 10.26               |
| Cellulose-acetate-propionate polymer:     |                     |
| description of                            | 10.11               |
| properties of                             | 10.28               |
| Cellulose nitrate polymer:                |                     |
| description of                            | 10.11               |
| properties of                             | 10.28               |
| Cellulose triacetate                      | 10.10               |
| Cellulosic polymers:                      |                     |
| description of                            | 10.10               |
| properties of                             | 10.26               |
| Celsius to Fahrenheit conversion factors  | 2.54                |
| Centered period, use of                   | 3.2                 |
| Centistokes, conversion factors           | 2.82                |
| Cerium:                                   |                     |
| bond dissociation energies                | 4.43                |
| equations and equivalents for             | 11.66               |
| gravimetric factors                       | 11.47               |
| Cesium:                                   |                     |
| bond dissociation energies                | 4.44                |
| gravimetric factors                       | 11.47               |
| Chain compounds, formulas for             | 3.2                 |
| Chain-transfer agents for polymers        | 10.4                |
| Characteristic of a common logarithm      | 2.102               |
| Characteristic low-mass neutral fragments |                     |
| from the molecular ion                    | 7.127               |
| Charge numbers in inorganic formulas      | 3.4                 |
| Charge-to-mass ratio for electron         | 2.4                 |
| Charles' law                              | 5.169               |
| Chemical Abstracts indexing system        | 1.49                |
| Chemical blowing agents for polymers      | 10.6                |
| Chemical nomenclature:                    |                     |
| inorganic                                 | 3.1                 |
| organic                                   | 1.2                 |
| Chemical reactions, symbols, SI units     |                     |
| and definitions                           | 2.7                 |
| Chemical resistance:                      |                     |
| or polymers                               | 10.64               |
| of rubbers                                | 10.65               |
| Chemical shifts:                          |                     |
| of boron-11                               | 7.111               |
| of carbon-13                              | 7.99                |
| attached to a double bond                 | 7.103               |
| in carbonyl groups                        | 7.106               |
| in substituted benzenes                   | 7.104               |
| in substituted pyridines                  | 7.105               |
| of fluorine-19                            | 7.117               |
| of nitrogen-15                            | 7.112               |
| of phosphorus-31                          | 7.119               |

| <b><u>Index Terms</u></b>                                    | <b><u>Links</u></b> |
|--------------------------------------------------------------|---------------------|
| Chemical shifts: ( <i>Cont.</i> )                            |                     |
| of protons in methine and methylene groups, estimation of    | 7.94                |
| of protons, in monosubstituted benzene                       | 7.96                |
| of residual protons in incompletely deuterated solvents      | 7.98                |
| of silicon-29                                                | 7.118               |
| Chemical structures:                                         |                     |
| of crystals                                                  | 4.58                |
| of ion-exchange resins                                       | 11.32               |
| of polymers                                                  | 10.8    10.58       |
| of rubbers                                                   | 10.58               |
| Chemical symbols and definitions                             | 2.6                 |
| Chemicals:                                                   |                     |
| common reactive and incompatible                             | 11.130              |
| flammable                                                    | 11.136              |
| recommended for refrigerated storage                         | 11.136              |
| which polymerize or decompose on extended refrigeration      | 11.136              |
| Chi square distribution                                      | 2.128               |
| percentiles of                                               | 2.129               |
| Chiral compounds, sequence rules for                         | 1.44                |
| Chirality and optical activity                               | 1.45                |
| Chloride, formation constants with                           | 8.83                |
| Chlorinated polyester polymer, properties of                 | 10.28               |
| Chlorinated poly(vinyl chloride), properties of              | 10.56               |
| Chlorine:                                                    |                     |
| bond dissociation energies                                   | 4.44                |
| gravimetric factors                                          | 11.47               |
| overpotential of                                             | 8.140               |
| solubility in water at various temperatures                  | 5.4                 |
| Chlorosulfonated polyethylene                                | 10.58               |
| Chromatographic behavior of solutes                          | 11.27               |
| Chromatographic solvents                                     | 11.16               |
| Chromatography, symbols and definitions for                  | 2.8                 |
| Chromium:                                                    |                     |
| bond dissociation energies                                   | 4.44                |
| gravimetric factors                                          | 11.47               |
| Chromophores, electronic absorption                          |                     |
| bands for                                                    | 7.19                |
| Circle, properties of                                        | 2.110               |
| Citrate reference pH buffer solution at various temperatures | 8.105               |
| Citric acid, formation constants with                        | 8.90                |
| Clapeyron equation                                           | 6.3                 |
| Clausius-Clapeyron equation                                  | 6.3                 |
| Cleaning solutions for fritted glassware                     | 11.69               |
| Cobalt:                                                      |                     |
| bond dissociation energies                                   | 4.33                |
| gravimetric factors                                          | 11.48               |
| Coefficient of linear expansion, of polymers                 | 10.22               |
| Coefficient of variation, in statistics                      | 2.114               |
| Coefficient of viscosity                                     | 5.137               |

| <b><u>Index Terms</u></b>                                        | <b><u>Links</u></b> |
|------------------------------------------------------------------|---------------------|
| Collective inorganic names                                       | 3.4                 |
| Colloid chemistry, symbols, SI units, and definitions for        | 2.10                |
| Colloids, protective                                             | 11.95               |
| Column efficiency                                                | 11.27               |
| Column selectivity factor ( <i>see Relative retention</i> )      |                     |
| Combustible mixtures in air                                      | 5.139               |
| Commercial plastics, properties of                               | 10.22               |
| Common logarithms                                                | 2.102               |
| Complexometric titrations                                        | 11.89               |
| indicators for                                                   | 11.96               |
| Compressibility factor, in gas chromatography                    | 11.26               |
| critical                                                         | 6.134               |
| Compressibility of water                                         | 5.156               |
| Compressive modulus of polymers                                  | 10.22               |
| Compressive strength, rupture, of polymers                       | 10.22               |
| Compton wavelength of electron, neutron, and proton              | 2.4                 |
| Conductance                                                      | 8.157               |
| of electrolyte solution, defined                                 | 8.169               |
| relations in                                                     | 8.168               |
| Conductivities, equivalent, of electrolytes in aqueous solutions | 8.163               |
| Conductivity:                                                    |                     |
| defined                                                          | 8.168               |
| equivalent                                                       | 8.169               |
| electrical, of various pure liquids                              | 8.161               |
| of standard potassium chloride solutions                         | 8.160               |
| of water at various temperatures                                 | 8.168               |
| Conductivity, thermal:                                           |                     |
| of elements                                                      | 4.2                 |
| of gases at various temperatures                                 | 5.148               |
| of liquids at various temperatures                               | 5.151               |
| of solids                                                        | 5.154               |
| Cone, volume and area of                                         | 2.112               |
| Confidence level and limits                                      | 2.124               |
| Configuration, electronic, of elements                           | 4.2                 |
| Conformational isomers                                           | 1.39                |
| Conjunctive nomenclature                                         | 1.21                |
| Constants, fundamental                                           | 2.117               |
| Control charts                                                   | 2.137               |
| Conversion factors                                               | 2.35                |
| temperature                                                      | 2.54                |
| Cooling mixtures                                                 | 11.3                |
| Coordination bonds, dipole moments                               | 4.54                |
| Coordination compounds, inorganic nomenclature of                | 3.10                |
| Copolymerization                                                 | 10.3                |
| Copper:                                                          |                     |
| bond dissociation energies                                       | 4.44                |
| gravimetric factors                                              | 11.49               |
| Copper vs. copper-nickel alloy thermocouple                      | 11.140 11.149       |

| <u>Index Terms</u>                                                     | <u>Links</u> |     |
|------------------------------------------------------------------------|--------------|-----|
| Correction for solvents in ultraviolet-visible region                  | 7.23         |     |
| Coupling agents for polymers                                           | 10.4         |     |
| Covalent radii of elements                                             | 4.35         |     |
| Critical compressibility factor, defined                               | 6.143        |     |
| Critical density                                                       | 6.143        |     |
| Critical phenomena                                                     | 6.142        |     |
| Critical pressure                                                      | 6.142        |     |
| of elements and compounds                                              | 6.142        |     |
| Critical temperature, of elements and compounds                        | 6.141        |     |
| Critical volume, of elements and compounds                             | 6.142        |     |
| Critical X-ray absorption energies                                     | 7.8          |     |
| Cross-linked polymer, defined                                          | 10.3         |     |
| Cross section, thermal neutron absorption, of nuclides                 | 4.59         |     |
| Crucibles used for fusions                                             | 11.70        |     |
| Cryoscopic constants                                                   | 11.4         |     |
| Crystal lattice types                                                  | 4.57         |     |
| Crystalline polymers                                                   | 10.2         |     |
| Crystal structures, in inorganic nomenclature                          | 3.10         |     |
| Crystals, analyzing, for X-ray spectroscopy                            | 7.15         |     |
| Cube, area and volume of                                               | 2.112        |     |
| Cubic crystal lattices                                                 | 4.57         |     |
| Cubical coefficients of thermal expansion                              | 11.105       |     |
| Cumulated double bonds:                                                |              |     |
| infrared frequencies of                                                | 7.49         |     |
| Raman frequencies of                                                   | 7.77         |     |
| Curium, bond dissociation energy                                       | 4.44         |     |
| Curve fitting                                                          | 2.133        |     |
| Cyanato type compounds, nomenclature of                                | 1.36         |     |
| Cyanide, formation constants with                                      | 8.84         |     |
| Cyclic compounds, conformations of                                     | 1.41         |     |
| Cyclic hydrocarbons with side chains, nomenclature of                  | 1.11         |     |
| Cyclic ring systems:                                                   |              |     |
| carbon-13 chemical shifts in                                           | 7.100        |     |
| nitrogen-15 chemical shifts in                                         | 7.113        |     |
| proton chemical shifts in                                              | 7.93         |     |
| Cyclohexanol, binary azeotropes with                                   | 5.70         |     |
| Cylinder, volume and area of                                           | 2.112        |     |
| Dalton's law of partial pressures                                      | 5.170        |     |
| Dative bonds, dipole moments                                           | 4.54         |     |
| Debye-Hückel equation                                                  | 8.2          | 8.5 |
| Decay of radionuclides                                                 | 4.59         |     |
| Definitions of physical and chemical quantities                        | 2.6          |     |
| Deflection temperature of polymers under flexural load                 | 10.22        |     |
| Degree Celsius ( <i>see Celsius to Fahrenheit conversion factors</i> ) |              |     |

**Index Terms****Links**

|                                                                              |        |      |
|------------------------------------------------------------------------------|--------|------|
| Degree Fahrenheit ( <i>see Fahrenheit to Celsius conversion factors</i> )    |        |      |
| Degree kelvin                                                                | 2.3    |      |
| Degree of ionic character of bonds                                           | 4.29   |      |
| Degrees of freedom, in statistics                                            | 2.123  |      |
| Deionizer, in flame photometry                                               | 7.41   |      |
| Demasking                                                                    | 11.93  |      |
| Demasking agents (table)                                                     | 11.100 |      |
| Density:                                                                     |        |      |
| of aqueous glycerol solutions                                                | 5.138  |      |
| conversion to degrees Baumé and Twaddell                                     | 2.85   |      |
| critical                                                                     | 6.143  |      |
| determined, with pycnometer                                                  | 5.89   |      |
| with plummet or sinker                                                       | 5.89   |      |
| of elements                                                                  | 3.12   |      |
| hydrometers and relation between scales                                      | 2.66   |      |
| of inorganic compounds                                                       | 3.12   |      |
| of mercury                                                                   | 5.87   |      |
| of moist air                                                                 | 5.88   |      |
| of organic compounds                                                         | 1.76   |      |
| of solvents                                                                  | 11.18  |      |
| and specific gravity                                                         | 2.66   | 5.87 |
| of sucrose solutions                                                         | 5.138  |      |
| of water                                                                     | 5.85   |      |
| Derivatives and differentiation                                              | 2.104  |      |
| Desiccants                                                                   | 11.5   |      |
| Detection limits, atomic absorption and atomic emission                      | 7.29   |      |
| Determinative errors                                                         | 2.118  |      |
| Deuterated solvents, chemical shifts:                                        |        |      |
| of carbon-13                                                                 | 7.110  |      |
| of residual protons                                                          | 7.98   |      |
| Deuterium oxide, vapor pressure of                                           | 5.30   |      |
| Dew point readings and relative humidity                                     | 11.9   |      |
| Diallyl phthalate molding polymers, properties of                            | 10.26  |      |
| Diallyl phthalate polymers                                                   | 10.10  |      |
| Diamagnetic shielding factor, spherical water molecule                       | 2.4    |      |
| 1,2-Diarninocyclohexane-N,N,N',N'-tetra-acetic acid formation constants with | 8.90   |      |
| Diastereomers                                                                | 1.39   |      |
| Diatomic molecules:                                                          |        |      |
| binding energies of                                                          | 4.41   |      |
| bond lengths                                                                 | 4.29   |      |
| Dibenzoylmethane, formation constants with                                   | 8.91   |      |
| Dichromate, volumetric factors for                                           | 11.79  |      |
| Dielectric constant:                                                         |        |      |
| discussion of                                                                | 5.137  |      |
| of inorganic compounds                                                       | 5.130  |      |
| of organic compounds                                                         | 5.105  |      |
| of water at various temperatures                                             | 5.134  |      |
| of polymers                                                                  | 10.22  |      |

| <b><u>Index Terms</u></b>                                             | <b><u>Links</u></b> |
|-----------------------------------------------------------------------|---------------------|
| Dielectric strength of polymers                                       | 10.22               |
| Dienes, absorption maxima of                                          | 7.19                |
| Dienones, absorption wavelength of                                    | 7.22                |
| Differentiation, rules for                                            | 2.104               |
| 4,5-Dihydroxybenzene-1,3-disulfonic acid,<br>formation constants with | 8.91                |
| Dimensionless quantities, symbols and<br>definitions                  | 2.22                |
| 2,3-Dimercaptopropan-1-ol, formation<br>constants with                | 8.92                |
| Dimethylglyoxime, formation constants with                            | 8.92                |
| Dimethylsulfoxide, pKa values in                                      | 8.81                |
| Dipole moments                                                        | 4.53                |
| discussion of                                                         | 5.136               |
| of inorganic compounds                                                | 5.130               |
| of organic compounds                                                  | 5.105               |
| 2,2-Dipyridyl, formation constants with                               | 8.92                |
| Dispersion of data, measures of                                       | 2.121               |
| Dissipation (power) factor of polymers                                | 10.22               |
| Dissociation energy of diatomic molecules                             | 4.41                |
| Distribution coefficient in ion exchange                              | 11.39               |
| Distribution curve, normal                                            | 2.119               |
| Distribution of measurements                                          | 2.118               |
| Distribution ratio, symbols and definitions for                       | 2.8                 |
| Double bonds:                                                         |                     |
| cumulated:                                                            |                     |
| infrared frequencies of                                               | 7.49                |
| Raman frequencies of                                                  | 7.77                |
| estimation of chemical shift of protons<br>attached                   | 7.95                |
| infrared red frequencies of                                           | 7.49                |
| protons attached, estimation of chemical<br>shift                     | 7.95                |
| Raman frequencies of                                                  | 7.79                |
| Double-bond radii, of elements                                        | 4.35                |
| Drying agents                                                         | 11.5                |
| Drying and humidification                                             | 11.5                |
| Duane-Hunt equation                                                   | 7.39                |
| Durometer hardness of rubbers                                         | 10.63               |
| Dynamic viscosity                                                     | 5.137               |
| Dysprosium, bond dissociation energies                                | 4.44                |
| Ebullioscopic constants                                               | 11.13               |
| ED PM rubber                                                          | 10.60               |
| EDTA complex, formation constants of                                  | 11.97               |
| EDTA, values of $\alpha_4$ at various pH values                       | 11.97               |
| Effective ionic radii in aqueous solutions                            | 8.4                 |
| Effective plate number                                                | 11.28               |
| Einstein equation                                                     | 7.38                |
| Elastomeric fibers                                                    | 10.18               |
| Elastomers, defined                                                   | 10.2                |
| Electric quadrupole moment of elements                                | 7.89                |
| Electrical conductivity of pure liquids                               | 8.161               |
| Electrical properties of polymers                                     | 10.22               |



| <b><u>Index Terms</u></b>                                         | <b><u>Links</u></b> |
|-------------------------------------------------------------------|---------------------|
| Electrical resistivity of elements                                | 4.2                 |
| Electric current                                                  | 2.3                 |
| Electricity, symbols, SI units, and definitions                   | 2.11                |
| Electrochemistry, symbols, SI units,<br>and definitions           | 2.12                |
| Electrode potentials                                              | 8.124               |
| Electrodes, reference, potential of                               | 8.113               |
| Electrolytes, equivalent conductivities in<br>aqueous solutions   | 8.163               |
| Electromagnetic radiation                                         | 7.38                |
| symbols, SI units, and definitions for                            | 2.13                |
| Electrometric measurement of pH                                   | 8.115               |
| Electron affinities, of elements, molecules,<br>and radicals      | 4.24                |
| Electron magnetic moment                                          | 2.4                 |
| Electron radius, classical                                        | 2.4                 |
| Electron rest mass                                                | 2.4                 |
| Electronegative constituents, in inorganic<br>formulas            | 3.3                 |
| Electronegativity                                                 | 4.28                |
| of elements (table)                                               | 4.29                |
| Electronic absorption bands for chromophores                      | 7.19                |
| Electronic configuration of elements                              | 4.2                 |
| Electrothermal atomic absorption, detection<br>limits of elements | 7.29                |
| Elementary charge                                                 | 2.4                 |
| Elements:                                                         |                     |
| abundance of naturally occurring isotopes                         | 4.81                |
| atom radius of                                                    | 4.29                |
| atomic number of                                                  | 4.2                 |
| density of                                                        | 3.12                |
| effective ionic radii                                             | 4.30                |
| electrical resistivity of                                         | 4.2                 |
| electron affinities of                                            | 4.24                |
| electronegativities of                                            | 4.29                |
| electronic configuration and properties                           | 4.1                 |
| ionization energy                                                 | 4.6                 |
| isotopes of naturally occurring                                   | 4.81                |
| linear thermal expansion of                                       | 4.2                 |
| magnetic moment of                                                | 7.89                |
| names and symbols for                                             | 3.3                 |
| nuclear properties of                                             | 4.42                |
| potentials of                                                     | 8.124               |
| quadrupole moment of                                              | 7.89                |
| sensitive emission lines of                                       | 7.34                |
| standard stock solutions                                          | 11.107              |
| symbols of                                                        | 4.2                 |
| thermal conductivity of                                           | 4.2                 |
| work functions of                                                 | 4.80                |
| X-ray filters for                                                 | 7.14                |
| Ellipse, area of                                                  | 2.111               |
| Ellipsoid, area and volume of                                     | 2.113               |
| Elongation, at break of polymers                                  | 10.22               |
| ultimate, of rubbers                                              | 10.60               |

| <u>Index Terms</u>                                                 | <u>Links</u> |      |
|--------------------------------------------------------------------|--------------|------|
| Emergent stem correction of thermometers                           | 11.150       |      |
| Emission energies, X-ray                                           | 7.10         |      |
| Emission limits of elements                                        | 7.29         |      |
| Emission spectra, X-ray                                            | 7.3          |      |
| Emission wavelengths, of fluorescent compounds                     | 7.25         |      |
| Empirical formula index of organic compounds                       | 1.58         |      |
| Enantiomers                                                        | 1.46         |      |
| Enclosing marks, use in inorganic formulas                         | 3.2          |      |
| Energy equivalents                                                 | 2.4          |      |
| Energy of ionization of molecular and radical species              | 4.8          |      |
| Engler degrees                                                     | 2.82         |      |
| Enones, absorption wavelength of                                   | 7.22         |      |
| Enthalpies:                                                        |              |      |
| of inorganic compounds                                             | 6.81         |      |
| of organic compounds                                               | 6.5          |      |
| Enthalpy:                                                          |              |      |
| of formation                                                       | 6.2          |      |
| of ions                                                            | 4.8          |      |
| of melting:                                                        |              |      |
| of inorganic compounds                                             | 6.124        |      |
| of organic compounds                                               | 6.51         |      |
| of sublimation                                                     | 6.3          |      |
| of inorganic compounds                                             | 6.124        |      |
| of organic compounds                                               | 6.51         |      |
| of a system                                                        | 6.4          |      |
| of vaporization                                                    | 6.3          |      |
| of inorganic compounds                                             | 6.124        |      |
| of organic compounds                                               | 6.51         |      |
| Enthalpy change of bonds ( <i>see Bond dissociation energies</i> ) |              |      |
| Entropies:                                                         |              |      |
| of inorganic compounds                                             | 6.81         |      |
| of melting                                                         | 6.4          | 6.51 |
| of organic compounds                                               | 6.5          |      |
| of sublimation                                                     | 6.4          |      |
| of vaporization                                                    | 6.4          |      |
| Entropy of a system                                                | 6.5          |      |
| Epichlorohydrin rubber                                             | 10.59        |      |
| Epoxy casting resins, properties of                                | 10.30        |      |
| Epoxy polymers                                                     | 10.11        |      |
| Epoxy resins, properties of                                        | 10.28        |      |
| Epoxy silicone polymers, properties of                             | 10.48        |      |
| Equations of state for real gases                                  | 5.170        |      |
| Equivalent conductances:                                           |              |      |
| of hydrogen ion at various temperatures                            | 8.168        |      |
| of hydroxyl ion at various temperatures                            | 8.168        |      |
| Equivalent conductivity:                                           |              |      |
| defined                                                            | 8.169        |      |
| of electrolytes in aqueous solutions                               | 8.163        |      |
| Equivalent ionic conductances, limiting                            | 8.157        |      |

| <b><u>Index Terms</u></b>                                                             | <b><u>Links</u></b> |
|---------------------------------------------------------------------------------------|---------------------|
| Equivalent weights for redox determinations<br>(See also <i>Titrimetric factors</i> ) | 11.84               |
| Erbium, bond dissociation energies                                                    | 4.45                |
| gravimetric factors                                                                   | 11.49               |
| Eriochrome Black T, formation constants with                                          | 8.92                |
| Error curve                                                                           | 2.119               |
| Error probability, in statistics                                                      | 2.123               |
| Errors in quantitative analysis                                                       | 2.118               |
| Esters:                                                                               |                     |
| binary azeotropes with                                                                | 5.59                |
| infrared frequencies of                                                               | 7.50                |
| of inorganic acids                                                                    | 3.9                 |
| nomenclature of                                                                       | 1.36                |
| Raman frequencies of                                                                  | 7.78                |
| Ethane, solubility in water at various<br>temperatures                                | 5.4                 |
| 1,2-Ethanediol, binary azeotropes with                                                | 5.72                |
| 1,2-Ethanediol monoacetate, binary<br>azeotropes with                                 | 5.73                |
| Ethanol:                                                                              |                     |
| binary azeotropes with                                                                | 5.66                |
| pKa values in                                                                         | 8.81                |
| ternary azeotropes with                                                               | 5.77                |
| vapor permeability for polymers                                                       | 10.69               |
| Ethanolamine, formation constants with                                                | 8.93                |
| Ethanol-water mixtures, freezing point of                                             | 5.83                |
| Ethers:                                                                               |                     |
| binary azeotropes with                                                                | 5.61                |
| infrared frequencies of                                                               | 7.58                |
| Raman frequencies of                                                                  | 7.85                |
| 2-Ethoxyethanol, binary azeotropes with                                               | 5.72                |
| Ethyl acetate, vapor permeability for<br>polymers                                     | 10.69               |
| Ethyl cellulose polymer:                                                              |                     |
| description of                                                                        | 10.11               |
| properties of                                                                         | 10.28               |
| Ethylene, solubility in water at various<br>temperatures                              | 5.4                 |
| Ethylene-chlorotrifluoroethylene copolymer:                                           |                     |
| description of                                                                        | 10.13               |
| properties of                                                                         | 10.32               |
| Ethylene glycol-water mixtures, freezing<br>point of                                  | 5.84                |
| Ethylene-propylene-diene rubber                                                       | 10.60               |
| Ethylene-tetrafluoroethylene copolymer                                                | 10.13               |
| Ethylene-vinyl acetate copolymer,<br>properties of                                    | 10.44               |
| Ethylenediamine, formation constants with                                             | 8.93                |
| Ethylenediamine-N,N,N',N'-tetraacetic acid,<br>formation constants with               | 8.93                |
| Ethylenediaminetetraacetic acid, values of<br>$\alpha_4$ at various pH                | 11.91               |
| Europium, bond dissociation energies                                                  | 4.45                |

| <b><u>Index Terms</u></b>                                  | <b><u>Links</u></b> |
|------------------------------------------------------------|---------------------|
| Excitation wavelengths of fluorescent compounds            | 7.25                |
| Expansion in series                                        | 2.115               |
| Explosive limits of combustible mixtures in air            | 5.139               |
| Exponential series                                         | 2.115               |
| Eykman equation                                            | 5.135               |
| <i>F</i> statistic (tables)                                | 2.131               |
| <i>F</i> test for equality of variances                    | 2.130               |
| Face-centered lattices                                     | 4.57                |
| Fahrenheit to Celsius conversion factors                   | 2.54                |
| Faraday constant                                           | 2.5                 |
| Fats, properties of                                        | 10.69               |
| Fatty oil hydrometer                                       | 2.67                |
| Fehling's solution                                         | 11.114              |
| Filters, membrane for X-rays                               | 11.70               |
|                                                            | 7.132               |
| Fine structure constant                                    | 2.5                 |
| First radiation constant                                   | 2.5                 |
| Flame atomic absorption, detection limits of elements      | 7.29                |
| Flame emission, detection limits of elements               | 7.29                |
| Flame retardants for polymers                              | 10.5                |
| Flammable chemicals                                        | 11.115              |
| Flammable limits of combustible mixtures in air            | 5.139               |
| Flash point of organic compounds                           | 1.76                |
| Flasks, volumetric, tolerances for                         | 11.102              |
| Flexural modulus of polymers                               | 10.22               |
| Flexural strength, rupture, of polymers                    | 10.22               |
| Fluidity, definition of                                    | 5.133               |
| Fluorescence                                               | 7.25                |
| laws of                                                    | 7.38                |
| plasma atomic, detection limits of elements                | 7.29                |
| quantum yield values                                       | 7.28                |
| standards                                                  | 7.28                |
| Fluorescent compounds, excitation and emission wavelengths | 7.25                |
| Fluorescent indicators for acid-base titrations            | 8.120               |
| Fluoride, formation constants with                         | 8.84                |
| Fluorinated ethylene-propylene resin:                      |                     |
| description of                                             | 10.12               |
| properties of                                              | 10.32               |
| Fluorine:                                                  |                     |
| bond dissociation energies                                 | 4.45                |
| equations and equivalents for                              | 11.68               |
| gravimetric factors                                        | 11.49               |
| Fluorine-carbon spin coupling constants                    | 7.109               |
| Fluorine-19 to fluorine-19 spin coupling constants         | 7.118               |
| Fluorine-19 chemical shifts                                | 7.117               |

| <u>Index Terms</u>                                                  | <u>Links</u> |
|---------------------------------------------------------------------|--------------|
| Fluorocarbon polymers:                                              |              |
| description of                                                      | 10.12        |
| properties of                                                       | 10.30        |
| Fluxes for sample decomposition                                     | 11.70        |
| Foaming agents for polymers                                         | 10.5         |
| Foams, polyurethane                                                 | 10.18        |
| Formation, enthalpy of                                              | 6.2          |
| Formation constants of metal complexes                              | 8.82         |
| with inorganic ligands                                              | 8.83         |
| with organic ligands                                                | 8.88         |
| Formic acid, binary azeotropes with                                 | 5.62         |
| Formula weights:                                                    |              |
| of inorganic compounds                                              | 3.14         |
| of organic compounds                                                | 1.76         |
| Formulas:                                                           |              |
| of inorganic compounds                                              | 3.14         |
| of organic compounds                                                | 1.76         |
| of plastic materials                                                | 10.8         |
| writing, of inorganic compounds                                     | 3.1          |
| <i>(See also Nomenclature)</i>                                      |              |
| Fortin barometer                                                    | 2.70         |
| Fourier's series                                                    | 2.116        |
| Fragmentation patterns in mass spectrometry                         | 7.126        |
| Free radicals, writing formula for                                  | 3.2          |
| Freedom, degrees of, in statistics                                  | 2.123        |
| Freezing mixtures                                                   | 5.83         |
| Freezing point, molecular lowering of                               | 11.4         |
| Frequency, defined                                                  | 7.38         |
| Fritted glassware:                                                  |              |
| cleaning solutions for                                              | 11.69        |
| pore sizes of                                                       | 11.71        |
| Functional class names in radicofunctional nomenclature             | 1.22         |
| Functional groups, in ion-exchange resins                           | 11.32        |
| nomenclature of                                                     | 1.23         |
| Functional organic compounds, nomenclature of                       | 1.17         |
| Fundamental physical constants                                      | 2.3          |
| Fused polycyclic hydrocarbons, nomenclature of                      | 1.6          |
| Fusion, heats of (see Heats of melting)                             |              |
| <i>g</i> factor (Landé) for free electron                           | 2.5          |
| Gadolinium, bond dissociation energies                              | 4.45         |
| gravimetric factors                                                 | 11.50        |
| Gallium, bond dissociation energies                                 | 4.27         |
| Gas (ideal), molar equivalent at various pressures and temperatures | 2.88         |
| Gas chromatography:                                                 |              |
| McReynolds' constants                                               | 11.21        |
| stationary phases                                                   | 11.21        |
| Gas constant                                                        | 2.5          |

**Index Terms****Links**

Gases:

equations of state for 5.170

permeability constants of polymers and  
rubbers 10.66

physical chemistry equations for 5.169

reduction to standard temperature and  
pressure 2.91

solubility in water at various temperatures 5.3

thermal conductivities at various  
temperatures 5.148

Van der Waals' constants 5.157

velocity of 5.171

Gaussian distribution curve 2.119

Geometric mean of set of numbers 2.118 2.119

Geometrical isomerism 1.43

Geometrical isomers, sequences rules for 1.44

Geometry, molecular 4.56

Germanium, bond dissociation energies 4.45

gravimetric factors 11.50

Gibbs energies of formation:

of inorganic compounds 6.81

of organic compounds 6.5

Glycerol-water mixtures:

density and viscosity of 5.138

freezing point of 5.85

Glycine, formation constants with 8.94

Gold, bond dissociation energies 4.45

gravimetric factors 11.50

Graft copolymers 10.3

Graham's law of diffusion, of gases 5.171

Grating equation 7.40

Gravimetric analysis, reagents for 11.67

Gravimetric factors 11.41

Gravitational constant 2.4

Gravity-latitude corrections for barometer 2.75

Greek alphabet 2.25

GRN rubber 10.59

Group dipole moments 4.54

Group refractions 5.136

Gutta percha 10.58

Hafnium, bond dissociation energies 4.45

Haggenmacher equation 6.3

Half-lives, of nuclides 4.59

Half-wave potentials, voltammetric:

of inorganic materials 8.141

of organic materials 8.146

Haloalkanes, Raman frequencies of 7.80

Halogen compounds:

infrared frequencies of 7.62

Raman frequencies of 7.86

Halogen-carbon bond lengths 4.36

Halogen derivatives (organic),

nomenclature of 1.31

| <b><u>Index Terms</u></b>                        | <b><u>Links</u></b> |       |
|--------------------------------------------------|---------------------|-------|
| Halogenated hydrocarbons, binary azeotropes with | 5.59                |       |
| Hammett equation                                 | 9.2                 |       |
| Hammett substituent constants                    | 9.2                 |       |
| Hardness:                                        |                     |       |
| of polymers                                      | 10.22               |       |
| of rubbers                                       | 10.63               |       |
| Hartree energy                                   | 2.5                 |       |
| Heat capacities:                                 |                     |       |
| of inorganic compounds                           | 6.81                | 6.124 |
| of organic compounds                             | 6.5                 | 6.51  |
| Heat capacity of any phase                       | 6.3                 |       |
| Heating baths                                    | 11.15               |       |
| Heating temperatures of precipitates             | 11.72               |       |
| Heats of fusion ( <i>see Heats of melting</i> )  |                     |       |
| Heats of melting:                                |                     |       |
| of inorganic compounds                           | 6.124               |       |
| of organic compounds                             | 6.51                |       |
| Heats of sublimation:                            |                     |       |
| of inorganic compounds                           | 6.124               |       |
| of organic compounds                             | 6.51                |       |
| Heats of vaporization:                           |                     |       |
| of inorganic compounds                           | 6.124               |       |
| of organic compounds                             | 6.51                |       |
| Helium:                                          |                     |       |
| gas permeability of polymers and rubbers         | 10.66               |       |
| solubility in water at various temperatures      | 5.8                 |       |
| Henry's law for gases                            | 5.172               |       |
| Heteroaromatics, primary absorption bands of     | 7.23                |       |
| Heteroatomic inorganic anions, nomenclature of   | 3.5                 |       |
| Heterocyclic rings:                              |                     |       |
| carbon-13 chemical shifts                        | 7.100               | 7.101 |
| proton chemical shifts, in saturated             | 7.93                |       |
| in unsaturated                                   | 7.94                |       |
| Raman frequencies of                             | 7.87                |       |
| Heterocyclic systems, nomenclature of            | 1.11                |       |
| Hexagonal crystal lattice                        | 4.57                | 4.58  |
| Hexane, vapor permeability for polymers          | 10.69               |       |
| High-density polyethylene, properties of         | 10.44               |       |
| High performance liquid chromatography           | 11.30               |       |
| Hittorf transport numbers                        | 8.169               |       |
| HPLC, typical performances                       | 11.31               |       |
| Humidity, relative:                              |                     |       |
| from dew points                                  | 11.9                |       |
| from wet and dry bulb thermometer readings       | 11.8                |       |
| Humidity, solutions for maintaining constant     | 11.6                | 11.7  |
| Hybrid bonds                                     | 4.56                |       |
| Hydrocarbon ring assemblies, nomenclature of     | 1.10                |       |
| Hydrocarbons:                                    |                     |       |
| binary azeotropes with                           | 5.61                |       |
| halogenated, binary azeotropes with              | 5.59                |       |

**Index Terms****Links**

## Hydrogen:

|                                             |       |
|---------------------------------------------|-------|
| binary inorganic compounds,                 | 3.5   |
| nomenclature of                             |       |
| bond dissociation energies                  | 4.46  |
| bond lengths with other elements            | 4.39  |
| gas permeability of polymers and rubbers    | 10.66 |
| gravimetric factors                         | 11.50 |
| infrared frequencies of single bonded       | 7.42  |
| overpotential of                            | 8.140 |
| solubility in water at various temperatures | 5.4   |

## Hydrogen-carbon:

|                                       |             |
|---------------------------------------|-------------|
| bond lengths                          | 4.37        |
| single bonds, infrared frequencies of | 7.41        |
| Raman frequencies of                  | 7.71        |
| spin coupling constants               | 7.107 7.108 |

## Hydrogen bromide, solubility in water at various temperatures

5.8

## Hydrogen chloride, solubility in water at various temperatures

5.8

## Hydrogen ion, equivalent conductance at various temperatures

8.168

*(See also pH)*

## Hydrogen-nitrogen, infrared absorption

|                         |       |
|-------------------------|-------|
| frequencies             | 7.46  |
| spin coupling constants | 7.122 |
| Raman frequencies       | 7.74  |

## Hydrogen overpotential

8.140

## Hydrogen sulfide, solubility in water at various temperatures

5.6

## Hydrometer conversion table

2.85

## Hydrometers

2.66

## Hydroxide, formation constants with

8.84

## N-(2-Hydroxyethyl)ethylenediamine-

N,N,N'-triacetic acid, formation constants with 8.95

## 6-Hydroxy-2-methylquinoline, formation constants with

8.95

## Hydroxyl group:

|                         |      |
|-------------------------|------|
| infrared frequencies of | 7.44 |
| Raman frequencies of    | 7.74 |

## Hydroxyl ion, equivalent conductance at various temperatures

8.168

## Hydroxylamines, nomenclature of

1.31

## 8-Hydroxyquinoline-5-sulfonic acid, formation constants with

8.95

## Hypotheses about means

2.126

## Ice, vapor pressure of

5.26

## ICP, detection limits of elements

7.29

Ignition temperature, *(see Autoignition)*

## Imides, infrared frequencies of

7.53

## Imines:

|                         |      |      |
|-------------------------|------|------|
| infrared frequencies of | 7.46 | 7.54 |
| nomenclature of         | 1.32 |      |



| <b><u>Index Terms</u></b>                                        | <b><u>Links</u></b> |
|------------------------------------------------------------------|---------------------|
| Impact strength (Izod) of polymers                               | 10.22               |
| Inches mercury, conversion to other pressure units               | 2.87                |
| Inches water, conversion to other pressure units                 | 2.87                |
| Incompatible and reactive chemicals                              | 11.130              |
| Indeterminate errors                                             | 2.118               |
| Indicators:                                                      |                     |
| for acid-base titrations                                         | 8.116               |
| for complexometric titrations                                    | 11.96               |
| for oxidation-reduction titrations                               | 8.122               |
| preparation of                                                   | 11.109              |
| Indium, bond dissociation energies                               | 4.47                |
| gravimetric factors                                              | 11.51               |
| Induction coupled plasma, detection limits of elements           | 7.29                |
| Inductive effect of a substituent                                | 9.2                 |
| Infrared spectroscopy                                            | 7.41                |
| Infrared transmission characteristics of solvents                | 7.68                |
| Infrared transmitting materials                                  | 7.67                |
| Inhibitors for polymers                                          | 10.6                |
| Inorganic acids, binary azeotropes with                          | 5.58                |
| Inorganic compounds:                                             |                     |
| nomenclature of                                                  | 3.1                 |
| physical constants of                                            | 3.12                |
| physical properties of                                           | 5.130               |
| proton-transfer reactions of                                     | 8.18                |
| solubilities in water at various temperatures                    | 5.9                 |
| solubility rules for                                             | 11.105              |
| synonyms and mineral names                                       | 3.62                |
| thermodynamic properties of                                      | 6.81                |
| vapor pressures of                                               | 5.31                |
| Inorganic ions:                                                  |                     |
| infrared frequencies of                                          | 7.64                |
| limiting equivalent conductances                                 | 8.157               |
| Integrals                                                        | 2.105               |
| Intercept of best-fit line, errors in                            | 2.35                |
| International temperature scale, fixed points in                 | 11.138              |
| International Union of Pure and Applied Chemistry, nomenclature: |                     |
| of inorganic compounds                                           | 3.1                 |
| of organic compounds                                             | 1.1                 |
| Interplanar spacings                                             | 7.13                |
| for $K\alpha_1$ radiation, of $\alpha$ -quartz                   | 7.14                |
| for $K\alpha_1$ radiation, of silicon                            | 7.14                |
| Interplanar spacings, standards for                              | 7.13                |
| Iodate, formation constants with                                 | 8.85                |
| Iodide, formation constants with                                 | 8.85                |

**Index Terms****Links**

Iodine:

|                            |       |
|----------------------------|-------|
| bond dissociation energies | 4.47  |
| gravimetric factors        | 11.51 |
| overpotential of           | 8.140 |
| titrimetric factors        | 11.78 |

Iodine titrant, volumetric factors for 11.78

Iodine value:

|                  |       |
|------------------|-------|
| of fats and oils | 10.69 |
| of waxes         | 10.72 |

Ion-exchange 11.37

Ion-exchange resins, guide to 11.32

Ion product constant of water at various temperatures 8.6

Ionic character of a bond 4.29

Ionic conductances, limiting equivalent 8.157

Ionic crystal lattices 4.57

Ionic equivalent conductivity, defined 8.169

Ionic mobility, defined 8.169

Ionic radii 4.34

|                      |      |     |
|----------------------|------|-----|
| in aqueous solutions | 8.4  | 8.5 |
| of elements          | 4.29 |     |

Ionic strength 8.2

Ionization energy:

|                      |     |
|----------------------|-----|
| of elements          | 4.6 |
| of molecular species | 4.8 |
| of radical species   | 4.8 |

Ionization of metals in a plasma 7.40

Ionized emission lines of elements 7.34

Ionomer polymers 10.17

Ions:

|                                  |       |
|----------------------------------|-------|
| activity coefficients in water   | 8.3   |
| enthalpy of formation            | 6.2   |
| limiting equivalent conductances | 8.157 |

Indium, bond dissociation energies 4.47

Iron:

|                            |       |
|----------------------------|-------|
| bond dissociation energies | 4.47  |
| gravimetric factors        | 11.51 |

Iron vs. copper-nickel alloy thermocouple 11.139 11.140 11.144

Isobutyric acid, binary azeotropes with 5.65

Isopolyanions, inorganic, nomenclature of 3.7

Isotactic arrangement 10.3

Isotopic abundances:

|                              |       |       |
|------------------------------|-------|-------|
| naturally occurring elements | 4.81  | 7.123 |
| of selected elements         | 7.124 |       |

Isotopically labeled compounds, nomenclature of 3.4

ITS-90, fixed points in 11.137 11.138

IUPAC (*see International Union of Pure and Applied Chemistry*)

Izod impact strength of polymers 10.22

Josephson frequency-voltage ratio 2.5

Joule-Thompson coefficient for real gases 5.172

| <b><u>Index Terms</u></b>                               | <b><u>Links</u></b> |      |
|---------------------------------------------------------|---------------------|------|
| KA <sub>1</sub> lines, mass absorption coefficients for | 7.16                |      |
| Kelvin, definition of                                   | 2.3                 |      |
| Kelvin scale, conversion to other<br>thermometer scales | 2.66                |      |
| Ketenes, nomenclature of                                | 1.32                |      |
| Ketones:                                                |                     |      |
| binary azeotropes with                                  | 5.61                | 5.74 |
| infrared frequencies of                                 | 7.51                |      |
| nomenclature of                                         | 1.32                |      |
| Raman frequencies of                                    | 7.78                |      |
| Kilogram, definition of                                 | 2.3                 |      |
| Kinematic viscosity                                     | 5.138               |      |
| Kinetics, symbols, SI units, and<br>definitions for     | 2.14                |      |
| Kovats retention indices                                | 11.26               |      |
| Krypton:                                                |                     |      |
| bond dissociation energies                              | 4.47                |      |
| solubility in water at various temperatures             | 5.8                 | 3.4  |
| Laboratory solutions                                    | 11.106              |      |
| Lactams, nomenclature of                                | 1.34                |      |
| Lactic acid, formation constants with                   | 8.96                |      |
| Lactides, nomenclature of                               | 1.34                |      |
| Lactims, nomenclature of                                | 1.34                |      |
| Lactometers                                             | 2.67                |      |
| Lactones:                                               |                     |      |
| infrared frequencies of                                 | 7.50                |      |
| nomenclature of                                         | 1.34                |      |
| Ladder polymer, defined                                 | 10.3                |      |
| Lanthanum, bond dissociation energies                   | 4.47                |      |
| Laser lines of argon-ion plasma                         | 7.89                |      |
| Latitude-gravity corrections for barometry              | 2.75                |      |
| Lattice types of crystal structures                     | 4.57                |      |
| Laws of photometry                                      | 7.38                |      |
| Lead:                                                   |                     |      |
| bond dissociation energies                              | 4.47                |      |
| gravimetric factors                                     | 11.52               |      |
| Least squares or best-fit line                          | 2.133               |      |
| Length                                                  | 2.3                 |      |
| Level of significance, in statistics                    | 2.124               |      |
| Ligand names, abbreviations for                         | 3.11                |      |
| Ligands:                                                |                     |      |
| abbreviations for names                                 | 3.11                |      |
| attachment points of                                    | 3.10                |      |
| inorganic, nomenclature of                              | 3.10                |      |
| Limiting equivalent ionic conductances                  | 8.157               |      |
| Linear free energy relationships                        | 9.2                 |      |
| Linear polymers, defined                                | 10.3                |      |
| Linear thermal expansion of elements                    | 4.2                 |      |
| Liquids:                                                |                     |      |
| electrical conductivity of pure                         | 8.161               |      |
| thermal conductivities of                               | 5.150               |      |

| <b><u>Index Terms</u></b>                        | <b><u>Links</u></b> |
|--------------------------------------------------|---------------------|
| Lithium:                                         |                     |
| bond dissociation energies                       | 4.47                |
| gravimetric factors                              | 11.53               |
| Logarithmic series                               | 2.115               |
| Logarithms                                       | 2.102               |
| Lorentz and Lorenz equation                      | 5.135               |
| Low-density polyethylene, properties of          | 10.44               |
| Lubricants for polymers                          | 10.6                |
| Luminous intensity                               | 2.3                 |
| Lutetium, bond dissociation energies             | 4.48                |
| Magnesium:                                       |                     |
| bond dissociation energies                       | 4.48                |
| gravimetric factors                              | 11.53               |
| Magnesium chloride brines, freezing              |                     |
| point of                                         | 5.86                |
| Magnetic flux quantum                            | 2.5                 |
| Magnetic moment:                                 |                     |
| of elements                                      | 7.89                |
| of protons in water                              | 2.5                 |
| Magnetism, symbols, SI units, and                |                     |
| definitions for                                  | 2.10                |
| Manganese:                                       |                     |
| bond dissociation energies                       | 4.48                |
| gravimetric factors                              | 11.54               |
| Mantissa of a common logarithm                   | 2.102               |
| Masking agents                                   | 11.92               |
| (table)                                          | 11.98               |
| Mass                                             | 2.3                 |
| Mass absorption coefficients for $K\alpha_1$ and |                     |
| $WLa_1$ lines                                    | 7.15                |
| Mass differences, exact                          | 7.124               |
| Mass spectra, correlation with molecular         |                     |
| structure                                        | 7.123               |
| Mathematical symbols and abbreviations           | 2.23                |
| Maximum allowable exposure limits for            |                     |
| gases and vapors                                 | 11.121              |
| Maximum recommended service temperature          |                     |
| of polymers                                      | 10.22               |
| McReynold's constants in gas                     |                     |
| chromatography                                   | 11.21               |
| Mean free path of gases                          | 5.171               |
| Mean ionic activity coefficient                  | 8.2                 |
| Mean of set of numbers                           | 2.111               |
| Measurements, distribution of                    | 2.111               |
| Measures of dispersion of data                   | 2.114               |
| Mechanical properties of polymers                | 10.22               |
| Mechanics, symbols, SI units, and                |                     |
| definitions for                                  | 2.15                |
| Median of set of numbers                         | 2.118               |
| Medium-density polyethylene, properties of       | 10.44               |
| Melamine formaldehyde polymer:                   |                     |
| description of                                   | 10.13               |
| properties of                                    | 10.32               |

**Index Terms****Links**

|                                                       |        |      |
|-------------------------------------------------------|--------|------|
| Melmine phenolic, woodflour-cellulose, filled plastic |        |      |
| properties of                                         | 10.34  |      |
| Melting, enthalpy of                                  | 6.4    |      |
| of inorganic compounds                                | 6.112  |      |
| of organic compounds                                  | 6.51   |      |
| Melting point:                                        |        |      |
| of inorganic compounds                                | 3.14   |      |
| molecular lowering of                                 | 11.4   |      |
| of organic compounds                                  | 1.76   |      |
| of waxes                                              | 10.72  |      |
| Melting temperature of polymers                       | 10.22  |      |
| Membrane filters                                      | 11.70  |      |
| Mercury:                                              |        |      |
| bond dissociation energies                            | 4.48   |      |
| density at various temperatures                       | 5.87   |      |
| gravimetric factors                                   | 11.55  |      |
| vapor pressure of                                     | 5.24   |      |
| Metal-carbon bond lengths                             | 4.38   |      |
| Metal complexes, formation constants of               | 8.83   |      |
| Metal salts of organic acids, solubilities in         |        |      |
| water at various temperatures                         | 5.9    |      |
| Metastable peaks, use in mass spectrometry            | 7.125  |      |
| Meter, definition of                                  | 2.3    |      |
| Methacrylate monomers                                 | 10.10  |      |
| Methane, solubility in water at various               |        |      |
| temperatures                                          | 5.6    |      |
| Methanol:                                             |        |      |
| binary azeotropes with                                | 5.66   |      |
| pKa values in                                         | 8.81   |      |
| ternary azeotropes with                               | 5.77   | 5.82 |
| Methanol-water mixtures, freezing point of            | 5.83   |      |
| Methine protons:                                      |        |      |
| chemical shift of                                     | 7.92   |      |
| estimation of chemical shift for                      | 7.94   |      |
| 3-Methyl-1-butanol:                                   |        |      |
| binary azeotropes with                                | 5.70   |      |
| ternary azeotropes with                               | 5.78   |      |
| 2-Methyl-1-propanol, ternary azeotropes with          | 5.78   |      |
| 2-Methyl-2-propanol:                                  |        |      |
| binary azeotropes with                                | 5.69   |      |
| ternary azeotropes with                               | 5.78   |      |
| Methyl protons, chemical shift of                     | 7.92   |      |
| Methylene protons:                                    |        |      |
| chemical shift of                                     | 7.92   |      |
| estimation of chemical shift for                      | 7.94   |      |
| Micropipets, tolerances for                           | 11.103 |      |
| Millimeters mercury, conversion to other              |        |      |
| pressure units                                        | 2.87   |      |
| Millimeters water, conversion to other                |        |      |
| pressure units                                        | 2.87   |      |
| Mineral names of inorganic compounds                  | 3.61   |      |
| Minimum radius ratio of hybrid bonds                  | 4.56   |      |
| Mixed acid-base indicators                            | 8.118  |      |

| <b><u>Index Terms</u></b>                                                | <b><u>Links</u></b> |      |
|--------------------------------------------------------------------------|---------------------|------|
| Mode for set of numbers                                                  | 2.118               |      |
| Moist air:                                                               |                     |      |
| density of                                                               | 5.88                |      |
| refractive index of                                                      | 5.135               |      |
| Molal values from molar values                                           | 2.88                |      |
| Molar absorptivity, defined                                              | 7.39                |      |
| Molar equivalent of 1 liter of gas at various pressures and temperatures | 2.88                |      |
| Molar refraction                                                         | 5.135               |      |
| Molar values, conversion to molal                                        | 2.88                |      |
| Molar volume, ideal gas                                                  | 2.5                 |      |
| Mole, definition of                                                      | 2.3                 |      |
| Molecular formula:                                                       |                     |      |
| of inorganic compounds                                                   | 3.2                 | 3.14 |
| of organic compounds                                                     | 1.76                |      |
| Molecular geometry                                                       | 4.56                |      |
| Molecular lowering of the melting point                                  | 11.4                |      |
| Molecular structure, determination from mass spectra                     | 7.123               |      |
| Molecular weight:                                                        |                     |      |
| determined by lowering of melting point                                  | 11.4                |      |
| determined by molecular elevation of boiling point                       | 11.13               |      |
| Molecules:                                                               |                     |      |
| electron affinities of                                                   | 4.25                |      |
| ionization energy of                                                     | 4.8                 |      |
| symbols, SI units and definitions                                        | 2.6                 |      |
| Molybdenum:                                                              |                     |      |
| bond dissociation energies                                               | 4.48                |      |
| gravimetric factors                                                      | 11.55               |      |
| Monoclinic crystal lattices                                              | 4.57                | 4.58 |
| Monocyclic aliphatic and aromatic hydrocarbons, nomenclature of          | 1.5                 |      |
| Multiplicative prefixes in inorganic nomenclature                        | 3.10                |      |
| Multiplying affixes                                                      | 1.21                |      |
| Must hydrometer                                                          | 2.68                |      |
| Naperian base (e)                                                        | 2.117               |      |
| Naphthalenes, Raman frequencies of                                       | 7.82                |      |
| Natural abundance:                                                       |                     |      |
| of elements                                                              | 7.89                |      |
| of nuclides                                                              | 4.59                | 7.89 |
| Natural rubber:                                                          |                     |      |
| description of                                                           | 10.58               |      |
| properties of                                                            | 10.63               |      |
| synthetic                                                                | 10.60               |      |
| Naturally occurring isotopes, relative abundance of                      | 4.81                |      |
| NBR rubber                                                               | 10.59               |      |
| NBS (see NIST, National Institute for Science and Technology)            |                     |      |
| Near infrared region, absorption frequencies in                          | 7.64                |      |
| Neodymium, bond dissociation energies                                    | 4.48                |      |

| <u>Index Terms</u>                                           | <u>Links</u>         |
|--------------------------------------------------------------|----------------------|
| Neon-neon bond dissociation energy                           | 4.48                 |
| Neon, solubility in water at various temperatures            | 5.8                  |
| Neoprene                                                     | 10.60                |
| Neptunium-oxygen bond dissociation energy                    | 4.48                 |
| Neutral inorganic radicals, nomenclature of                  | 3.5                  |
| Neutron rest mass                                            | 2.4                  |
| New York Board of Health lactometer                          | 2.67                 |
| Newtons per square meter, conversion to other pressure units | 2.87                 |
| Nickel:                                                      |                      |
| bond dissociation energies                                   | 4.48                 |
| gravimetric factors                                          | 11.55                |
| Nickel-chromium:                                             |                      |
| vs. copper-nickel alloys thermocouple                        | 11.139 11.140 11.143 |
| vs. nickel-aluminum alloys thermocouple                      | 11.139 11.140 11.145 |
| Niobium, gravimetric factors                                 | 11.56                |
| Niobium-oxygen bond dissociation energy                      | 4.48                 |
| NIST pH buffer solution                                      | 8.105 8.106          |
| Nitrate, formation constants with                            | 8.86                 |
| Nitric oxide, solubility in water at various temperatures    | 5.6                  |
| Nitrile polymers:                                            |                      |
| description of                                               | 10.13                |
| properties of                                                | 10.34                |
| Nitrile rubber                                               | 10.59                |
| Nitriles:                                                    |                      |
| binary azeotropes with                                       | 5.62                 |
| nomenclature of                                              | 1.35                 |
| Nitrilotriactic acid, formation constants with               | 8.96                 |
| Nitro compounds:                                             |                      |
| infrared frequencies of                                      | 7.55                 |
| Raman frequencies of                                         | 7.81                 |
| Nitrogen:                                                    |                      |
| bond dissociation energies                                   | 4.48                 |
| gas permeability of polymers and rubbers                     | 10.66                |
| gravimetric factors                                          | 11.56                |
| solubility in water at various temperatures                  | 5.6                  |
| Nitrogen-carbon:                                             |                      |
| bond lengths                                                 | 4.37                 |
| spin coupling constants                                      | 7.116                |
| Nitrogen-15:                                                 |                      |
| chemical shifts                                              | 7.112                |
| chemical shifts for standards                                | 7.115                |
| chemical shifts in monosubstituted pyridine                  | 7.115                |
| Nitrogen-14 NMR data ( <i>see Nitrogen-15</i> )              |                      |
| Nitrogen-fluorine spin coupling constants                    | 7.116                |
| Nitrogen-hydrogen bonds:                                     |                      |
| infrared frequencies                                         | 7.46                 |
| Raman frequencies of                                         | 7.75                 |
| Nitrogen-hydrogen spin coupling constants                    | 7.115                |
| Nitrogen-nitrogen double bonds, Raman frequencies of         | 7.81                 |
| Nitrogen-other elements bond lengths                         | 4.39                 |

| <b><u>Index Terms</u></b>                                  | <b><u>Links</u></b> |       |
|------------------------------------------------------------|---------------------|-------|
| Nitrogen-oxygen double bonds, Raman frequencies of         | 7.85                |       |
| 1-Nitroso-2-naphthol, formation constants with             | 8.97                |       |
| Nitrous oxide, solubility in water at various temperatures | 5.8                 |       |
| NMR frequency of elements for 1-kG field                   | 7.89                |       |
| NMR sensitivity at constant field of elements              | 7.89                |       |
| NMR spectroscopy                                           | 7.92                |       |
| Nomenclature:                                              |                     |       |
| of inorganic compounds                                     | 3.1                 |       |
| of organic compounds                                       | 1.1                 |       |
| Nonaqueous solvents:                                       |                     |       |
| pKa values in                                              | 8.81                |       |
| potential ranges in                                        | 8.80                |       |
| Nonfunctional organic compounds, nomenclature of           | 1.1                 |       |
| Normal distribution curve in statistics                    | 2.119               |       |
| Novolac resin, properties of                               | 10.11               | 10.30 |
| Nuclear magnetic resonance                                 | 7.89                |       |
| Nuclear magneton                                           | 2.5                 |       |
| Nuclear properties of elements                             | 4.58                | 7.89  |
| Nuclear reactions, symbols for                             | 2.8                 |       |
| Nuclear spin of elements                                   | 7.89                |       |
| Nuclides:                                                  |                     |       |
| capture cross section, thermal                             | 4.59                |       |
| natural abundance of                                       | 4.59                | 7.89  |
| properties of                                              | 4.58                |       |
| radiation emitted                                          | 4.59                |       |
| Numbering of organic compounds                             | 1.20                |       |
| Numerical prefixes                                         | 2.25                |       |
| Nylon II polymers:                                         |                     |       |
| description of                                             | 10.14               |       |
| properties of                                              | 10.38               |       |
| Nylon 6 polymers:                                          |                     |       |
| description of                                             | 10.14               |       |
| properties of                                              | 10.36               |       |
| Nylon 6/9 polymers:                                        |                     |       |
| description of                                             | 10.14               |       |
| properties of                                              | 10.38               |       |
| Nylon 6/6-nylon 6 copolymer, properties of                 | 10.36               |       |
| Nylon 6/6 polymers:                                        |                     |       |
| description of                                             | 10.14               |       |
| properties of                                              | 10.36               |       |
| Nylon 6/12 polymers:                                       |                     |       |
| description of                                             | 10.14               |       |
| properties of                                              | 10.38               |       |
| Nylon 12 polymer:                                          |                     |       |
| description of                                             | 10.14               |       |
| properties of                                              | 10.38               |       |
| Octahedral covalent radii of elements                      | 4.36                |       |
| Oils, properties of                                        | 10.69               |       |
| Oleometer                                                  | 2.68                |       |



| <b><u>Index Terms</u></b>                          | <b><u>Links</u></b> |       |
|----------------------------------------------------|---------------------|-------|
| One-tailed test, in statistics                     | 2.125               |       |
| Optical rotation                                   | 1.46                |       |
| Orbitals, hybridized                               | 4.56                |       |
| Ordinates and areas of normal distribution curve   | 2.119               |       |
| Organic acids:                                     |                     |       |
| binary azeotropes with                             | 5.58                | 5.62  |
| salts of, solubilities at various temperatures     | 5.9                 |       |
| Organic compounds:                                 |                     |       |
| dielectric constants                               | 5.105               |       |
| dipole moments                                     | 5.105               |       |
| empirical formula index of                         | 1.58                |       |
| half-wave potentials                               | 8.146               |       |
| physical properties of                             | 1.76                | 5.90  |
| proton-transfer reactions of                       | 8.24                |       |
| surface tensions                                   | 5.90                |       |
| thermodynamic properties of                        | 6.5                 | 6.51  |
| vapor pressures of                                 | 5.39                |       |
| viscosity of                                       | 5.90                |       |
| Organic ions, limiting equivalent conductances     | 8.157               |       |
| Organic radicals, names and formulas of            | 1.51                |       |
| Organic solvents arranged by boiling points        | 11.10               |       |
| Organosulfur halides, nomenclature of              | 1.38                |       |
| Orientation, spatial, of common hybrid bonds       | 4.56                |       |
| Orthorhombic crystal lattices                      | 4.57                | 4.58  |
| Osmium-oxygen bond dissociation energy             | 4.49                |       |
| Ostwald dilution law                               | 8.169               |       |
| Overpotentials of electrode reactions              | 8.140               |       |
| Oxalate, formation constants with                  | 8.97                |       |
| Oxidation numbers, in inorganic formulas           | 3.4                 |       |
| Oxidation-reduction indicators                     | 8.122               | 11.83 |
| Oxidation-reduction titrants                       | 11.82               |       |
| Oxidation-reduction titrations, equations for      | 11.84               |       |
| Oximes, infrared frequencies of                    | 7.54                |       |
| Oxygen:                                            |                     |       |
| bond dissociation energies                         | 4.49                |       |
| gas permeability of polymers and rubbers           | 10.66               |       |
| overpotential                                      | 8.140               |       |
| solubility in water at various temperatures        | 5.6                 |       |
| Oxygen-carbon bond lengths                         | 4.37                |       |
| Oxygen-hydrogen bonds, infrared frequencies        | 7.44                |       |
| Oxygen-other elements bond lengths                 | 4.29                |       |
| Ozone, solubility in water at various temperatures | 5.8                 |       |
| Palladium, gravimetric factors                     | 11.57               |       |
| -oxygen bond dissociation energy                   | 4.49                |       |
| Parabola, properties of                            | 2.111               |       |
| Parallelogram, area of                             | 2.109               |       |
| Particles, symbols for                             | 2.8                 |       |
| Partition ratio                                    | 11.28               |       |
| Pascals, conversion to other pressure units        | 2.87                |       |
| Path length, of cuvettes                           | 7.40                |       |
| PCTA copolyester                                   | 10.16               |       |

| <b><u>Index Terms</u></b>                                       | <b><u>Links</u></b> |       |
|-----------------------------------------------------------------|---------------------|-------|
| Peak asymmetry factor                                           | 11.28               | 11.29 |
| Percent absorption to absorbance, table                         | 2.96                |       |
| Percent humidity:                                               |                     |       |
| of calcium chloride solutions                                   | 11.7                |       |
| of sodium hydroxide solutions                                   | 11.7                |       |
| of sulfuric acid solutions                                      | 11.7                |       |
| at various temperatures for various solutions                   | 11.6                |       |
| Perfluoroalkoxy polymer:                                        |                     |       |
| description of                                                  | 10.12               |       |
| properties of                                                   | 10.30               |       |
| Permanganate, volumetric factors for                            | 11.86               |       |
| Permeability of vacuum                                          | 2.5                 |       |
| Peroxides:                                                      |                     |       |
| infrared frequencies of                                         | 7.58                |       |
| nomenclature of                                                 | 1.35                |       |
| pH buffer solutions, standard reference                         | 8.104               |       |
| pH measurement:                                                 |                     |       |
| of blood and biological materials                               | 8.106               |       |
| electrometric                                                   | 8.115               |       |
| in 50 weight percent methanol-water                             | 8.109               |       |
| pH range:                                                       |                     |       |
| of acid-base indicators                                         | 8.116               |       |
| of fluorescent indicators                                       | 8.120               |       |
| pH values:                                                      |                     |       |
| for buffer solutions in alcohol-water solvents                  | 8.109               |       |
| of solutions, calculation of approximate                        | 8.17                | 8.23  |
| 1,10-Phenanthroline, formation constants with                   | 9.98                |       |
| Phenol, binary azeotropes with                                  | 5.71                |       |
| Phenol-formaldehyde resin                                       | 10.14               |       |
| Phenolic polymers:                                              |                     |       |
| description of                                                  | 10.14               |       |
| properties of                                                   | 10.34               |       |
| Phenols:                                                        |                     |       |
| nomenclature of                                                 | 1.24                |       |
| retained trivial names of                                       | 1.25                |       |
| Phosphate reference pH buffer solutions at various temperatures | 8.105               |       |
| Phosphate-succinate reference pH buffer solution                | 8.108               |       |
| Phosphorus:                                                     |                     |       |
| bond dissociation energies                                      | 4.49                |       |
| gravimetric factors                                             | 11.57               |       |
| other elements bond lengths                                     | 4.40                |       |
| Phosphorus compounds:                                           |                     |       |
| infrared frequencies of                                         | 7.60                |       |
| nomenclature of                                                 | 1.36                |       |
| Phosphorus-31:                                                  |                     |       |
| chemical shifts                                                 | 7.119               |       |
| spin coupling constants                                         | 7.122               |       |
| Photometry, laws of                                             | 7.38                |       |
| Phthalate reference pH buffer solution at various temperatures  | 8.105               |       |
| Phthalic acid, formation constants with                         | 9.99                |       |

| <b><u>Index Terms</u></b>                               | <b><u>Links</u></b>  |
|---------------------------------------------------------|----------------------|
| Physical chemistry equations for gases                  | 5.169                |
| Physical constants, fundamental                         | 2.3                  |
| Physical properties:                                    |                      |
| of inorganic compounds                                  | 3.12                 |
| of organic compounds                                    | 1.76                 |
| of polymers                                             | 10.22                |
| Physical symbols and definitions                        | 2.6                  |
| pi ( $\pi$ ), value of                                  | 2.117                |
| Piperidine, formation constants with                    | 8.99                 |
| Pipet capacity tolerances                               | 11.103               |
| pKa values at various temperatures                      | 8.73                 |
| pKa values:                                             |                      |
| of acid-base indicators                                 | 8.116                |
| of inorganic materials                                  | 8.18                 |
| in nonaqueous solvents                                  | 8.81                 |
| of organic materials                                    | 8.24                 |
| pK <sub>a</sub> <sup>0</sup> values:                    |                      |
| for Hammett equation                                    | 9.7                  |
| for Taft equation                                       | 9.8                  |
| Planck constant                                         | 2.5                  |
| Planck radiation law                                    | 11.138               |
| Plane angle                                             | 2.3                  |
| Plant fats and oils, properties of                      | 10.70                |
| Plastic families (table)                                | 10.6                 |
| Plasticizers for polymers                               | 10.7                 |
| Plastics, commercial:                                   |                      |
| formulas and key properties of                          | 10.8                 |
| properties of commercial                                | 10.22                |
| Plate height                                            | 11.28                |
| Plate number                                            | 11.28                |
| Platinum:                                               |                      |
| bond dissociation energies                              | 4.44                 |
| gravimetric factors                                     | 11.58                |
| Platinum-10% rhodium alloy vs. platinum thermocouple    | 11.139 11.140 11.148 |
| Platinum-13% rhodium alloy vs. platinum thermocouple    | 11.139 11.140 11.147 |
| Platinum-30% rhodium vs. platinum-6% rhodium alloys     | 11.139               |
| Polyacrylate rubbers                                    | 10.59                |
| Poly(acrylic acid) and poly(methacrylic acid) copolymer | 10.9                 |
| Poly(acrylonitrile) polymers                            | 10.10                |
| Polyallomer polyolefin polymer, properties of           | 10.46                |
| Polyamide polymers:                                     |                      |
| description of                                          | 10.14                |
| properties of                                           | 10.36                |
| Poly(amide-imide) polymers:                             |                      |
| description of                                          | 10.15                |
| properties of                                           | 10.38                |
| Poly(aryl ether) polymer, properties of                 | 10.40                |
| Polyatomic inorganic anions,                            |                      |
| nomenclature of                                         | 3.7                  |
| Polybutadiene rubber                                    | 10.59                |

| <b><u>Index Terms</u></b>                                  | <b><u>Links</u></b> |
|------------------------------------------------------------|---------------------|
| Polybutylene polymers                                      | 10.17               |
| Polybutylene extrusion polymer, properties of              | 10.46               |
| Poly(butylene terephthalate) polymers:                     |                     |
| description of                                             | 10.15               |
| properties of                                              | 10.40               |
| Polycarbonate polymer:                                     |                     |
| description of                                             | 10.15               |
| properties of                                              | 10.40               |
| Polycarbonate-acrylonitrile-butadiene-styrene alloy        | 10.26               |
| Polychloroprene rubber                                     | 10.60               |
| Poly(chlorotrifluoroethylene) polymer:                     |                     |
| description of                                             | 10.12               |
| properties of                                              | 10.30               |
| Polycyclic hydrocarbons, fused, nomenclature of            | 1.6                 |
| Poly(1,4-cyclohexanedimethylene terephthalic acid) polymer | 10.16               |
| Polyester polymers                                         | 10.15    10.20      |
| Polyester thermoplastic elastomers, properties of          | 10.54               |
| Polyesters                                                 | 10.15    10.20      |
| Poly(ether sulfone) polymer, properties of                 | 10.52               |
| Polyethylene polymers:                                     |                     |
| description of                                             | 10.16               |
| properties of                                              | 10.44               |
| Poly(ethylene terephthalate) polymers:                     |                     |
| description of                                             | 10.15               |
| properties of                                              | 10.40               |
| Polygon, area and properties of                            | 2.110               |
| Polyhedra, area of surface and volume                      | 2.112               |
| Polyimide polymers:                                        |                     |
| description of                                             | 10.16               |
| properties of                                              | 10.42               |
| Polyisobutylene rubber                                     | 10.60               |
| Polyisoprene rubber                                        | 10.60               |
| Polymers:                                                  | 10.2                |
| additives to                                               | 10.4                |
| gas permeability of                                        | 10.66               |
| properties of commercial                                   | 10.22               |
| resistance to chemicals                                    | 10.64               |
| structural differences                                     | 10.3                |
| vapor permeability constants for                           | 10.69               |
| Poly(methyl acrylate)                                      | 10.9                |
| Poly(methyl methacrylate) polymer:                         |                     |
| description of                                             | 10.9                |
| properties of                                              | 10.24               |
| Poly(methylpentene) polymer:                               |                     |
| description of                                             | 10.16               |
| properties of                                              | 10.44               |
| Polyolefin polymers                                        | 10.16               |
| in elastomers                                              | 10.20               |
| properties of                                              | 10.44               |

| <b><u>Index Terms</u></b>                                               | <b><u>Links</u></b> |       |
|-------------------------------------------------------------------------|---------------------|-------|
| Polyolefin thermoplastic elastomers,<br>properties of                   | 10.54               |       |
| Poly(phenyl sulfone) polymer, properties of                             | 10.52               |       |
| Poly(phenylene sulfide) polymer:<br>description of                      | 10.17               |       |
| properties of                                                           | 10.46               |       |
| Polypropylene polymers:<br>description of                               | 10.17               |       |
| properties of                                                           | 10.46               |       |
| Polysiloxanes                                                           | 10.19               |       |
| Polystyrene polymers:<br>description of                                 | 10.19               |       |
| properties of                                                           | 10.48               |       |
| Polysulfide rubbers                                                     | 10.61               |       |
| Polysulfone polymers:<br>description of                                 | 10.20               |       |
| properties of                                                           | 10.52               |       |
| Poly(tetrafluoroethylene) polymer:<br>description of                    | 10.12               |       |
| properties of                                                           | 10.30               |       |
| Poly(vinyl acetate) polymer                                             | 10.21               |       |
| Poly(vinyl alcohol) polymer                                             | 10.21               |       |
| Poly(vinyl butyral) polymer:<br>description of                          | 10.21               |       |
| properties of                                                           | 10.56               |       |
| Poly(vinyl chloride):<br>description of                                 | 10.20               |       |
| properties of                                                           | 10.56               |       |
| Poly(vinyl chloride) and poly(vinyl acetate)<br>polymers, properties of | 10.54               |       |
| Poly(vinyl fluoride) polymer                                            | 10.13               |       |
| Poly(vinyl formal) polymer, properties of                               | 10.56               |       |
| Poly(vinylidene chloride) polymer:<br>description of                    | 10.21               | 10.58 |
| properties of                                                           | 10.56               |       |
| Poly(vinylidene fluoride) polymer:<br>description of                    | 10.13               |       |
| properties of                                                           | 10.32               |       |
| Polyurethane polymers:<br>description of                                | 10.18               |       |
| properties of                                                           | 10.48               |       |
| Pore sizes:<br>of fritted glassware                                     | 11.60               |       |
| of membrane filters                                                     | 11.60               |       |
| Potassium:<br>bond dissociation energies                                | 4.32                |       |
| gravimetric factors                                                     | 11.58               |       |
| Potassium dichromate, volumetric factors for                            | 11.79               |       |
| Potassium permanganate, volumetric<br>factors for                       | 11.80               |       |
| Potentials of elements and their compounds                              | 8.124               |       |
| Pounds per square inch, conversion to other<br>units                    | 2.87                |       |
| Praseodymium, bond dissociation energies                                | 4.49                |       |

**Index Terms****Links**

|                                                                                                  |       |      |
|--------------------------------------------------------------------------------------------------|-------|------|
| Precipitates, heating temperatures,<br>composition of weighing forms, and<br>gravimetric factors | 11.72 |      |
| Precipitation titrations                                                                         | 11.89 |      |
| indicators for                                                                                   | 11.94 |      |
| standard solutions for                                                                           | 11.95 |      |
| Prefixes:                                                                                        |       |      |
| numerical (multiplying)                                                                          | 2.25  |      |
| SI                                                                                               | 2.25  |      |
| use in inorganic formulas                                                                        | 3.2   |      |
| Pressure, altitude variation of                                                                  | 2.78  |      |
| Pressure conversion chart                                                                        | 2.87  |      |
| Pressure, critical                                                                               | 6.143 |      |
| Prestone-water mixtures, freezing point of                                                       | 5.84  |      |
| Primary standards:                                                                               |       |      |
| for acid-base titrations                                                                         | 11.74 |      |
| for precipitation titrations                                                                     | 11.94 |      |
| for redox titrations                                                                             | 11.82 |      |
| Prismoid, volume of                                                                              | 2.112 |      |
| Probability curve                                                                                | 2.119 |      |
| Promethium, bond dissociation energies                                                           | 4.50  |      |
| 1-Propanol, binary azeotropes with                                                               | 5.67  |      |
| 1-Propanol, ternary azeotropic mixtures                                                          | 5.77  |      |
| 2-Propanol, binary azeotropes with                                                               | 5.68  |      |
| 2-Propanol, ternary azeotropic mixtures                                                          | 5.77  |      |
| Properties of plastic materials                                                                  | 10.8  |      |
| Propionic acid:                                                                                  |       |      |
| binary azeotropes with                                                                           | 5.64  |      |
| ternary azeotropic mixtures                                                                      | 5.82  |      |
| Propylene glycol-water mixtures, freezing<br>point of                                            | 5.85  |      |
| Propylene-1,2-diamine, formation<br>constants with                                               | 8.99  |      |
| Protective colloids                                                                              | 11.95 |      |
| Proton chemical shifts:                                                                          | 7.92  |      |
| attached to a double bond                                                                        | 7.95  |      |
| in monosubstituted benzene                                                                       | 7.95  |      |
| of reference compounds                                                                           | 7.98  |      |
| Proton magnetic moment                                                                           | 2.5   |      |
| Proton magnetogyric ratio                                                                        | 2.5   |      |
| Proton resonance frequency per field in water                                                    | 2.5   |      |
| Proton rest mass                                                                                 | 2.5   |      |
| Proton spin coupling constants                                                                   | 7.97  |      |
| Proton-transfer reactions                                                                        | 8.17  |      |
| of inorganic materials                                                                           | 8.18  | 8.73 |
| in nonaqueous solvents                                                                           | 8.81  |      |
| of organic materials                                                                             | 8.24  |      |
| at various temperatures                                                                          | 8.73  |      |
| Protonated inorganic anions,<br>nomenclature of                                                  | 3.6   |      |
| Protons attached to double bond, estimation<br>of chemical shift of                              | 7.95  |      |
| Psi, conversion to other pressure units                                                          | 2.87  |      |
| Pyknometer, determinations with                                                                  | 5.89  |      |

| <b><u>Index Terms</u></b>                                | <b><u>Links</u></b> |
|----------------------------------------------------------|---------------------|
| Pyridine:                                                |                     |
| binary azeotropes with                                   | 5.75                |
| carbon-13 chemical shifts in substituted                 | 7.115               |
| formation constants with                                 | 8.99                |
| nitrogen-15 chemical shifts in monosubstituted           | 7.115               |
| Pyridine-2,6-dicarboxylic acid, formation constants with | 8.99                |
| 1-(2-Pyridylazo)-2-naphthol, formation constants with    | 8.100               |
| 4-(2-Pyridylazo)resorcinol, formation constants with     | 8.100               |
| Pyrocatechol-3,5-disulfonate, formation constants with   | 8.99                |
| Pyrophosphate, formation constants with                  | 8.86                |
| Quadratic mean of set of numbers                         | 2.119               |
| Quadrupole moment of elements                            | 7.89                |
| Quantum of circulation                                   | 2.5                 |
| Quantum-charge ratio                                     | 2.5                 |
| Quantum yield values, fluorescence                       | 7.28                |
| Quartz, interplanar spacings with K $\alpha$ 1 radiation | 7.14                |
| Quevenne lactometer                                      | 2.67                |
| $\delta$ -Quinolinol, formation constants with           | 8.101               |
| Radian, definition of                                    | 2.3                 |
| Radiation buffer                                         | 7.41                |
| Radiation:                                               |                     |
| electromagnetic, symbols, SI units, and definitions for  | 2.12                |
| emitted by radionuclides                                 | 4.59                |
| Radical species, ionization energy of                    | 4.8                 |
| Radicals:                                                |                     |
| electron affinities of                                   | 4.27                |
| from ring systems, nomenclature of                       | 1.10                |
| Radical functional nomenclature                          | 1.22                |
| Radioactivity from nuclides                              | 4.59                |
| Radium-chlorine bond dissociation energy                 | 4.50                |
| Radius ratio, minimum                                    | 4.56                |
| Radon, solubility in water at various temperatures       | 5.8                 |
| Raman frequencies:                                       |                     |
| of aromatic compounds                                    | 7.82                |
| of carbonyl bands                                        | 7.78                |
| of cumulated double bonds                                | 7.76                |
| of double bonds                                          | 7.79                |
| of ethers                                                | 7.85                |
| of halogen compounds                                     | 7.86                |
| of heterocyclic rings                                    | 7.87                |
| of single bonds to hydrogen and carbon                   | 7.71                |
| of sulfur compounds                                      | 7.84                |
| of triple bonds                                          | 7.76                |
| Raman spectroscopy                                       | 7.71                |
| Random errors                                            | 2.118               |

| <b><u>Index Terms</u></b>                                  | <b><u>Links</u></b> |       |
|------------------------------------------------------------|---------------------|-------|
| Rankine scale, conversion of                               | 2.66                |       |
| Ratio, electron-to-proton magnetic moments                 | 2.5                 |       |
| Rayon                                                      | 10.11               |       |
| Reaction parameters in Harnmett equation                   | 9.2                 | 9.7   |
| Reactive and incompatible chemicals                        | 11.130              |       |
| Reagents, preparation of                                   | 11.109              |       |
| Reaumur scale, conversion of                               | 2.66                |       |
| Rectangle, area of                                         | 2.109               |       |
| Reduced plate height                                       | 11.31               |       |
| Reduced velocity                                           | 11.31               |       |
| Redwood seconds at several temperatures                    | 2.82                |       |
| Reference compounds in NMR:                                |                     |       |
| proton chemical shifts of                                  | 7.98                |       |
| for nitrogen-15 chemical shifts                            | 7.115               |       |
| Reference electrodes                                       | 8.113               |       |
| Refractions, atomic and group (table)                      | 5.135               |       |
| molar                                                      | 5.135               |       |
| Refractive index:                                          |                     |       |
| of chromatographic solvents                                | 11.16               |       |
| discussion of                                              | 5.135               |       |
| of fats and oils                                           | 10.69               |       |
| of moist air                                               | 5.135               |       |
| of organic compounds                                       | 1.76                |       |
| of solvents                                                | 11.18               |       |
| of water at various temperatures                           | 5.134               |       |
| of waxes                                                   | 10.72               |       |
| Refrigerated storage, chemical                             |                     |       |
| recommended for                                            | 11.136              |       |
| Relative abundance of naturally occurring isotopes         | 4.81                |       |
| Relative humidity:                                         |                     |       |
| from dew point readings                                    | 11.9                |       |
| from wet and dry bulb thermometer readings                 | 11.8                |       |
| Relative retention                                         | 11.28               |       |
| Replacement nomenclature                                   | 1.22                |       |
| Residual protons (NMR) in incompletely deuterated solvents | 7.98                |       |
| Resistance, chemical:                                      |                     |       |
| of polymers                                                | 10.64               |       |
| of rubbers                                                 | 10.65               |       |
| Resistivity:                                               |                     |       |
| defined                                                    | 8.168               |       |
| electrical, of elements                                    | 4.2                 |       |
| ( <i>see also Conductivity</i> )                           |                     |       |
| Resolution                                                 | 11.28               | 11.29 |
| Resonance effect of a substituent                          | 9.2                 |       |
| Retention behavior of solutes in chromatography            | 11.27               |       |
| Retention time (or volume)                                 | 11.27               |       |
| Reversing a series                                         | 2.116               |       |
| Reynolds number                                            | 5.138               |       |



| <b><u>Index Terms</u></b>                     | <b><u>Links</u></b> |      |
|-----------------------------------------------|---------------------|------|
| Rho values:                                   |                     |      |
| for Hammett equation                          | 9.7                 |      |
| in nucleophilic substitutions                 | 9.8                 |      |
| for special reaction centers                  | 9.8                 |      |
| Rhodium:                                      |                     |      |
| bond dissociation energies                    | 4.50                |      |
| gravimetric factors                           | 11.60               |      |
| Rhombohedral crystal lattice                  | 4.57                | 4.58 |
| Ring assemblies of hydrocarbons,              |                     |      |
| nomenclature of                               | 1.10                |      |
| Ring systems, radicals from, nomenclature of  | 1.10                |      |
| Rockwell hardness of polymers                 | 10.22               |      |
| Root mean square                              | 2.119               |      |
| $RT/nF$ values at several temperatures        | 8.115               |      |
| Rubbers:                                      | 10.58               |      |
| gas permeability of                           | 10.66               |      |
| properties of natural and synthetic           | 10.63               |      |
| resistance to chemicals                       | 10.64               |      |
| Rubidium:                                     |                     |      |
| bond dissociation energies                    | 4.50                |      |
| gravimetric factors                           | 11.60               |      |
| Ruthenium, bond dissociation energies         | 4.51                |      |
| Rydberg constant                              | 2.5                 |      |
| Saccharometers                                | 2.68                |      |
| Saha equation                                 | 7.41                |      |
| Salicylaldehyde, formation constants with     | 8.101               |      |
| Salicylic acid, formation constants with      | 8.101               |      |
| Salinometer                                   | 2.68                |      |
| Salts:                                        |                     |      |
| of inorganic acids, nomenclature of           | 3.10                |      |
| of organic acids, nomenclature of             | 1.36                |      |
| Samarium, bond dissociation energies          | 4.50                |      |
| Sample decomposition, fluxes for              | 11.61               |      |
| Sample variance                               | 2.118               |      |
| SAN copolymers:                               |                     |      |
| description of                                | 10.20               |      |
| properties of                                 | 10.52               |      |
| Saponification value:                         |                     |      |
| of fats and oils                              | 10.69               |      |
| of waxes                                      | 10.72               |      |
| Saturated air, mass of water vapor in, at     |                     |      |
| various temperatures                          | 5.156               |      |
| Saturated heterocyclic ring systems, proton   |                     |      |
| NMR signal                                    | 7.93                |      |
| Saybolt universal viscosity at several        |                     |      |
| temperatures                                  | 2.82                |      |
| Scandium, bond dissociation energies          | 4.50                |      |
| Screens, see sieves                           |                     |      |
| Sea level, reduction of barometer readings to | 2.79                |      |
| Second, definition of                         | 2.3                 |      |
| Second radiation constant                     | 2.5                 |      |

| <b><u>Index Terms</u></b>                                                  | <b><u>Links</u></b> |
|----------------------------------------------------------------------------|---------------------|
| Selection rules:                                                           |                     |
| for parent heterocyclic system                                             | 1.15                |
| for principal alicyclic chain                                              | 1.18                |
| for principal ring system                                                  | 1.18                |
| Selectivity coefficients for ion-exchange resins                           | 11.37               |
| Selenium:                                                                  |                     |
| bond dissociation energies                                                 | 4.50                |
| gravimetric factors                                                        | 11.60               |
| Selenium-carbon bond lengths                                               | 4.38                |
| Self-ignition temperatures of combustible mixture in air                   | 5.139               |
| Sensitivity of elements at constant field (NMR)                            | 7.89                |
| Separation methods                                                         | 11.16               |
| Sequence rules, geometrical isomers and chiral compounds                   | 1.44                |
| Service temperature:                                                       |                     |
| of commercial plastics                                                     | 10.23               |
| of rubbers of commercial plastics                                          | 10.63               |
| Shore hardness:                                                            |                     |
| of polymers                                                                | 10.22               |
| of natural and synthetic rubbers                                           | 10.63               |
| SI prefixes                                                                | 2.24                |
| SI units:                                                                  |                     |
| base                                                                       | 2.3                 |
| definition of                                                              | 2.3                 |
| derived                                                                    | 2.4                 |
| supplementary                                                              | 2.3                 |
| Sieve openings                                                             | 11.137              |
| Sieve sizes, U.S. standard                                                 | 11.137              |
| Silica, solvent strength parameters                                        | 11.16               |
| Silicon:                                                                   |                     |
| bond dissociation energies                                                 | 4.50                |
| gravimetric factors                                                        | 11.61               |
| interplanar spacings with $K\alpha_1$ , radiation                          | 7.14                |
| Silicon compounds:                                                         |                     |
| infrared frequencies of                                                    | 7.61                |
| nomenclature of                                                            | 1.37                |
| Silicon-carbon bond lengths                                                | 4.38                |
| Silicone polymers, properties of                                           | 10.48               |
| Silicone rubbers                                                           | 10.61               |
| Silicones                                                                  | 10.18               |
| Silicon-other elements bond lengths                                        | 4.40                |
| Silicon-29 chemical shifts                                                 | 7.119               |
| Silver:                                                                    |                     |
| bond dissociation energies                                                 | 4.50                |
| gravimetric factors                                                        | 11.61               |
| Silver nitrate, volumetric factors for                                     | 11.81               |
| Silver/silver bromide reference electrode, EMF as function of temperature  | 8.113               |
| Silver/silver chloride reference electrode, EMF as function of temperature | 8.113               |
| Silver/silver iodide reference electrode, EMF as function of temperature   | 8.113               |

| <b><u>Index Terms</u></b>                     | <b><u>Links</u></b> |
|-----------------------------------------------|---------------------|
| Single-bond radii, of elements                | 4.35                |
| Single bonds between hydrogen and carbon:     |                     |
| infrared frequencies of                       | 7.41                |
| Raman frequencies of                          | 7.71                |
| Single bonds between hydrogen and oxygen,     |                     |
| infrared frequencies                          | 7.44                |
| Single bonds between hydrogen and nitrogen    | 7.46                |
| Single-bond radii, of elements                | 4.35                |
| Slope of best-fit line, errors in             | 2.135               |
| Sodium:                                       |                     |
| bond dissociation energies                    | 4.51                |
| gravimetric factors                           | 11.61               |
| Sodium chloride brines, freezing point of     | 5.86                |
| Sodium hydroxide solutions, percent           |                     |
| humidity of                                   | 11.7                |
| Sodium thiosulfate solution, volumetric       |                     |
| factors for                                   | 11.82               |
| Solid angle                                   | 2.3                 |
| Solid state, symbols, SI units, and           |                     |
| definitions for                               | 2.16                |
| Solidification point, of fats and oils        | 10.69               |
| Solids, thermal conductivities                | 5.154               |
| Solid state, symbols, SI units, and           |                     |
| definitions for                               | 2.16                |
| Solubility:                                   |                     |
| of gases in water at various temperatures     | 5.3                 |
| of inorganic compounds                        | 3.14                |
| in water at various temperatures              | 5.9                 |
| of organic compounds                          | 1.76                |
| Solubility products:                          | 8.6                 |
| at various temperatures                       | 8.73                |
| Solubility rules for inorganic compounds      | 11.105              |
| Solute band profile                           | 11.29               |
| Solutes, chromatographic behavior of          | 11.27               |
| Solutions for analytical use, preparation of  | 11.109              |
| Solvent strength parameter                    | 11.16               |
| Solvents:                                     |                     |
| acid-base, properties of                      | 8.90                |
| arranged by boiling points                    | 11.10               |
| of chromatographic interest                   | 11.16               |
| correction for in ultraviolet-visible region  | 7.23                |
| having the same refractive index and          |                     |
| same density                                  | 11.18               |
| infrared transmission characteristics         | 7.68                |
| positions of residual protons (NMR) in        |                     |
| incompletely deuterated                       | 7.98                |
| ultraviolet cutoffs of                        | 7.20                |
| Soxhlet lactometer                            | 2.67                |
| Space, symbols, SI units, and definitions for | 2.17                |
| Spatial orientation of common hybrid bonds    | 4.56                |
| Specialist nomenclature for heterocyclic      |                     |
| systems                                       | 1.11                |

| <b><u>Index Terms</u></b>                              | <b><u>Links</u></b> |
|--------------------------------------------------------|---------------------|
| Specific gravity:                                      | 5.87                |
| conversion to density                                  | 2.66                |
| corrections for buoyant effect of air                  | 5.89                |
| of fats and oils                                       | 10.69               |
| of polymers                                            | 10.22               |
| of rubbers                                             | 10.63               |
| of waxes                                               | 10.72               |
| Specific heat:                                         |                     |
| of any phase                                           | 6.4                 |
| of polymers                                            | 10.23               |
| ( <i>see also Heat capacities</i> )                    |                     |
| Specific refraction                                    | 5.135               |
| Specific resistance                                    | 8.168               |
| Specific rotation                                      | 1.47                |
| Spectrophotometry, laws of                             | 7.39                |
| Spectroscopic relationships                            | 7.38                |
| Spectroscopy, symbols, SI units, and                   |                     |
| definitions for                                        | 2.16                |
| Speed of light in vacuum                               | 2.5                 |
| Sphere, area and volume of                             | 2.112               |
| Spin coupling constants:                               |                     |
| carbon-carbon                                          | 7.108               |
| carbon-fluorine                                        | 7.109               |
| of carbon-hydrogen                                     | 7.107               |
| of carbon with nuclei other than hydrogen              | 7.110               |
| fluorine-fluorine                                      | 7.118               |
| nitrogen-fluorine                                      | 7.116               |
| nitrogen-hydrogen                                      | 7.115               |
| of phosphorus                                          | 7.122               |
| of protons                                             | 7.97                |
| Spin, nuclear, of elements                             | 7.89                |
| Sprayometer                                            | 2.68                |
| Stability constants ( <i>see Formation constants</i> ) |                     |
| Standard acceleration of free fall                     | 2.5                 |
| Standard atmosphere                                    | 2.5                 |
| Standard deviation:                                    |                     |
| of chromatographic band                                | 11.29               |
| in statistics                                          | 2.120               |
| Standard enthalpies for compounds                      | 6.2                 |
| Standardized variable                                  | 2.120               |
| Standard letter symbols                                | 2.26                |
| Standard stock solutions for elements                  | 11.107              |
| Standards:                                             |                     |
| for acid-base titrations                               | 11.74               |
| for fluorescence                                       | 7.28                |
| for precipitation titrations                           | 11.94               |
| for redox titrations                                   | 11.82               |
| States of aggregation, abbreviations for               | 2.7                 |
| Stationary phases in gas chromatography                | 11.21               |
| Statistical tables                                     | 2.117               |
| Stefan's law                                           | 7.39                |
| Stefan-Boltzmann constant                              | 2.5                 |
| Steradian, definition of                               | 2.3                 |
| Stereochemistry                                        | 1.39                |

| <b><u>Index Terms</u></b>                                    | <b><u>Links</u></b> |
|--------------------------------------------------------------|---------------------|
| Stereoisomers                                                | 1.39                |
| Stoichiometric proportions, in inorganic nomenclature        | 3.3                 |
| Straight-chain alkanes, names of                             | 1.2                 |
| Strontium:                                                   |                     |
| bond dissociation energies                                   | 4.51                |
| gravimetric factors                                          | 11.63               |
| Structural formulas ( <i>see Formulas</i> )                  |                     |
| Student t values (table)                                     | 2.124               |
| Student's distribution                                       | 2.123               |
| Styrene-acrylonitrile copolymers:                            |                     |
| description of                                               | 10.19               |
| properties of                                                | 10.52               |
| Styrene-butadiene copolymer, properties of                   | 10.52               |
| Styrene-butadiene rubber                                     | 10.61               |
| Styrene-butadiene-styrene block copolymers                   | 10.20               |
| Styrene-maleic acid copolymer, properties of                 | 10.42               |
| Styrenic polymers:                                           |                     |
| description of                                               | 10.19               |
| properties of                                                | 10.48               |
| Sublimation, enthalpy of:                                    | 6.3                 |
| of inorganic compounds                                       | 6.124               |
| of organic compounds                                         | 6.51                |
| Sublimation, entropy of                                      | 6.4                 |
| Substitution pattern of benzene ring:                        |                     |
| infrared frequencies                                         | 7.57                |
| Raman frequencies                                            | 7.82                |
| Substitutive nomenclature                                    | 1.17                |
| Succinic acid, formation constants with                      | 8.102               |
| Sucrose-water solutions, density and viscosity of            | 5.138               |
| Suffixes for specialist nomenclature of Heterocyclic systems | 1.12                |
| Sulfate, formation constants with                            | 8.86                |
| Sulfite, formation constants with                            | 8.87                |
| Sulfone polymers:                                            |                     |
| description of                                               | 10.20               |
| properties of                                                | 10.52               |
| Sulfones, nomenclature of                                    | 1.38                |
| Sulfonium compounds, nomenclature of                         | 1.38                |
| 5-Sulfosalicylic acid, formation constants with              | 8.102               |
| Sulfoxides, nomenclature of                                  | 1.38                |
| Sulfur acids, nomenclature of                                | 1.38                |
| Sulfur:                                                      |                     |
| bond dissociation energies                                   | 4.51                |
| -carbon bond lengths                                         | 4.38                |
| gravimetric factors                                          | 11.64               |
| -other elements bond lengths                                 | 4.40                |
| Sulfur compounds:                                            |                     |
| infrared frequencies of                                      | 7.59                |
| nomenclature of                                              | 1.37                |
| Raman frequencies of                                         | 7.84                |
| Sulfur dioxide, solubility in water at various temperatures  | 5.6                 |

| <b><u>Index Terms</u></b>                                        | <b><u>Links</u></b> |
|------------------------------------------------------------------|---------------------|
| Sulfuric acid solutions:                                         |                     |
| percent humidity of                                              | 11.7                |
| specific vapor pressures of                                      | 11.7                |
| Sultams, nomenclature of                                         | 1.39                |
| Sultones, nomenclature of                                        | 1.39                |
| Supercritical fluids, table                                      | 11.26               |
| Suppression of ionization in a plasma                            | 7.41                |
| Surface areas and volumes                                        | 2.109               |
| Surface chemistry, symbols, SI units,<br>and definitions for     | 2.10                |
| Surface tension:                                                 |                     |
| discussion of                                                    | 5.136               |
| of inorganic compounds                                           | 5.130               |
| of organic compounds                                             | 5.90                |
| of water at various temperatures                                 | 5.134               |
| Symbols:                                                         |                     |
| of elements                                                      | 4.2                 |
| mathematical                                                     | 2.23                |
| physical and chemical                                            | 2.6                 |
| standard letter                                                  | 2.26                |
| Symmetry in crystal structures                                   | 4.58                |
| Syndiotactic arrangement                                         | 10.3                |
| Synonyms of inorganic compounds                                  | 3.61                |
| Synthetic rubbers:                                               |                     |
| defined                                                          | 10.3                |
| natural                                                          | 10.60               |
| properties of                                                    | 10.63               |
| Systematic errors                                                | 2.118               |
| <br><i>t</i> , values of                                         | 2.124               |
| <i>t</i> test                                                    | 2.123               |
| Tacticity, defined                                               | 10.3                |
| Taft sigma values                                                | 9.2                 |
| Taft substituent constants                                       | 9.2                 |
| Tantalum:                                                        |                     |
| bond dissociation energies                                       | 4.51                |
| gravimetric factors                                              | 11.64               |
| Tartaric acid, formation constants with                          | 8.102               |
| Tartrate reference pH buffer solution at<br>various temperatures | 8.105               |
| Tellurium:                                                       |                     |
| bond dissociation energies                                       | 4.51                |
| gravimetric factors                                              | 11.64               |
| Temperature correction, for barometric<br>readings               | 2.72                |
| Temperature                                                      | 2.3                 |
| conversion between Celsius and<br>Fahrenheit scales              | 2.54                |
| critical                                                         | 6.141               |
| measurement of                                                   | 11.138              |
| Tensile modulus of polymers                                      | 10.22               |
| Tensile yield strength:                                          |                     |
| at break of polymers                                             | 10.22               |
| of natural and synthetic rubbers                                 | 10.63               |

**Index Terms****Links**

|                                                |        |        |        |
|------------------------------------------------|--------|--------|--------|
| Tension, aqueous ( <i>see Vapor pressure</i> ) |        |        |        |
| Terbium, bond dissociation energies            | 4.51   |        |        |
| Ternary azeotropic mixtures                    | 5.77   |        |        |
| containing water and alcohols                  | 5.77   |        |        |
| Tests of significance, in statistics           | 2.126  |        |        |
| Tetragonal crystal lattices                    | 4.53   | 4.57   |        |
| Tetraoxalate reference pH buffer solution      |        |        |        |
| at various temperatures                        | 8.105  |        |        |
| Thallium:                                      |        |        |        |
| bond dissociation energies                     | 4.51   |        |        |
| gravimetric factors                            | 11.65  |        |        |
| Theoretical plates                             | 11.28  |        |        |
| Thermal conductivity:                          | 5.148  |        |        |
| of elements                                    | 4.2    |        |        |
| of gases at various temperatures               | 5.148  |        |        |
| of liquids at various temperatures             | 5.151  |        |        |
| of polymers                                    | 10.23  |        |        |
| of solids                                      | 5.154  |        |        |
| Thermal expansion:                             |        |        |        |
| cubical coefficients of                        | 11.105 |        |        |
| linear, coefficient of, elements               | 4.2    |        |        |
| Thermal neutron absorption cross section       |        |        |        |
| of nuclides                                    | 4.59   |        |        |
| Thermal properties of polymers                 | 10.22  |        |        |
| Thermocouples                                  | 11.138 |        |        |
| Type B                                         | 11.139 |        |        |
| Type E                                         | 11.139 | 11.140 | 11.143 |
| Type I                                         | 11.139 | 11.140 | 11.144 |
| Type K                                         | 11.139 | 11.140 | 11.145 |
| Type N                                         | 11.139 | 11.140 | 11.146 |
| Type R                                         | 11.139 | 11.140 | 11.147 |
| Type S                                         | 11.139 | 11.140 | 11.148 |
| Type T                                         | 11.139 | 11.140 | 11.149 |
| Thermodynamic properties                       | 6.1    |        |        |
| Thermodynamics, symbols, SI units, and         |        |        |        |
| definitions for                                | 2.19   |        |        |
| Thermoelastic elastomers                       | 10.20  |        |        |
| Thermometer scales, conversion between         | 2.59   |        |        |
| Thermometers, correction for emergent stem     | 11.150 |        |        |
| Thermometry                                    | 11.137 |        |        |
| Thermoplastic elastomers:                      |        |        |        |
| defined                                        | 10.2   | 10.20  |        |
| properties of                                  | 10.54  |        |        |
| Thermoplastic polyester polymers               | 10.40  |        |        |
| Thermoplastic polyurethane elastomer,          |        |        |        |
| properties of                                  | 10.48  |        |        |
| Thermosetting alkyd polyesters, properties of  | 10.42  |        |        |
| Thermosetting polymers, defined                | 10.2   |        |        |
| Thiocyanate, formation constants with          | 8.87   |        |        |
| Thioesters and thioacids, infrared             |        |        |        |
| frequencies of                                 | 7.53   |        |        |
| Thioglycolic acid, formation constants with    | 8.103  |        |        |
| Thiophene, binary azeotropes with              | 5.76   |        |        |

| <b><u>Index Terms</u></b>                                    | <b><u>Links</u></b> |
|--------------------------------------------------------------|---------------------|
| Thiosulfate:                                                 |                     |
| formation constants with                                     | 8.87                |
| volumetric factors for                                       | 11.88               |
| Thiourea, formation constants with                           | 8.103               |
| Thomson cross section                                        | 2.5                 |
| Thorium:                                                     |                     |
| bond dissociation energies                                   | 4.51                |
| gravimetric factors                                          | 11.65               |
| Thoron, formation constant with                              | 8.103               |
| Threshold limit value (TLV) for gases and vapors             | 11.121              |
| Thullium, bond dissociation energies                         | 4.51                |
| Time:                                                        |                     |
| of analysis in chromatography                                | 11.31               |
| defined                                                      | 2.3                 |
| symbols, SI units, and definitions for                       | 2.17                |
| Tin:                                                         |                     |
| bond dissociation energies                                   | 4.51                |
| gravimetric factors                                          | 11.65               |
| Tiron, formation constants with                              | 8.91                |
| Titanium:                                                    |                     |
| bond dissociation energies                                   | 4.52                |
| gravimetric factors                                          | 11.65               |
| Titrimetric factors:                                         |                     |
| acids                                                        | 11.76               |
| bases                                                        | 11.77               |
| iodine                                                       | 11.78               |
| potassium dichromate                                         | 11.79               |
| potassium permanganate                                       | 11.80               |
| silver nitrate                                               | 11.81               |
| sodium thiosulfate                                           | 11.82               |
| Titrimetric solutions, standard:                             |                     |
| for acid-base titrations                                     | 11.84               |
| for elements                                                 | 11.107              |
| for precipitation titrations                                 | 11.94               |
| for redox titrations                                         | 11.82               |
| Tolerances:                                                  |                     |
| for analytical weights                                       | 11.71               |
| for burets                                                   | 11.103              |
| for pipets                                                   | 11.103              |
| for volumetric flasks                                        | 11.102              |
| Torsional asymmetry                                          | 1.47                |
| Torus, area and volume of                                    | 2.113               |
| Tralle hydrometer                                            | 2.68                |
| Transference numbers                                         | 8.169               |
| Transmittance:                                               |                     |
| to absorbance (table)                                        | 2.98                |
| defined                                                      | 7.39                |
| Transport properties, symbols, SI units, and definitions for | 2.21                |
| Trapezoid, area of                                           | 2.109               |
| Triangle, area of                                            | 2.109               |
| Triclinic crystal lattice                                    | 4.57                |
| Triethanolamine, formation constants with                    | 8.103               |



| <u>Index Terms</u>                             | <u>Links</u> |
|------------------------------------------------|--------------|
| Triethylenetetramine, formation                |              |
| constants with                                 | 8.103        |
| 1,1,1-Trifluoro-3,2'-thenoylacetone, formation |              |
| constants with                                 | 8.104        |
| Trigonometric functions:                       |              |
| of an angle                                    | 2.113        |
| functions, series for                          | 2.116        |
| Triple-bond radii, of elements                 | 4.35         |
| Triple bonds:                                  |              |
| infrared frequencies of                        | 7.47         |
| Raman frequencies of                           | 7.76         |
| Triple points of various materials             | 5.168        |
| Trivial names of heterocyclic systems for use  |              |
| in fusion names                                | 1.13         |
| Trouton's rule                                 | 6.3          |
| Tungsten:                                      |              |
| bond dissociation energies                     | 4.52         |
| gravimetric factors                            | 11.66        |
| Tungsten $L\alpha_1$ line, mass absorption     |              |
| coefficients for                               | 7.16         |
| Twaddell degrees:                              |              |
| conversion to degrees Baume                    | 2.85         |
| conversion to density                          | 2.85         |
| Twaddell hydrometer                            | 2.68         |
| Two-tailed test, in statistics                 | 2.125        |
| Ultraviolet-visible spectroscopy               | 7.19         |
| Ultraviolet cutoff:                            |              |
| of chromatographic solvents                    | 11.16        |
| of spectrograde solvents                       | 7.20         |
| Ultraviolet stabilizers for polymers           | 10.7         |
| Unit cells in crystal structures               | 4.59         |
| Unsaturated carbon-hydrogen bond, Raman        |              |
| frequencies                                    | 7.73         |
| Unsaturated polyester polymers                 | 10.16        |
| Unsaturated cyclic ring systems, carbon-13     |              |
| chemical shifts                                | 7.101        |
| Unsaturated heterocyclic ring systems, proton  |              |
| chemical shifts in                             | 7.94         |
| Uranium:                                       |              |
| bond dissociation energies                     | 4.52         |
| gravimetric factors                            | 11.66        |
| Urea formaldehyde resin                        | 10.21        |
| description of                                 | 10.58        |
| properties of                                  | 10.54        |
| Ureas, infrared frequencies of                 | 7.53         |
| Van der Waals' constants for gases             | 5.157        |
| Van der Waals' equation of state for gases     | 5.157 5.170  |
| Vanadium:                                      |              |
| bond dissociation energies                     | 4.52         |
| gravimetric factors                            | 11.66        |
| Vapor density, of gases                        | 5.171        |

| <b><u>Index Terms</u></b>                 | <b><u>Links</u></b> |
|-------------------------------------------|---------------------|
| Vaporization:                             |                     |
| enthalpy of                               | 6.3                 |
| of inorganic compounds                    | 6.124               |
| of organic compounds                      | 6.51                |
| entropy of                                | 6.4                 |
| Vapor permeability constants for polymers | 10.69               |
| Vapor-pressure equations                  | 5.29                |
| Vapor pressure:                           |                     |
| of ammonia (liquid)                       | 5.27                |
| of deuterium oxide                        | 5.30                |
| of ice                                    | 5.26                |
| of inorganic compounds                    | 5.31                |
| of mercury                                | 5.24                |
| of water                                  | 5.28                |
| of organic compounds                      | 5.39                |
| of solutions                              | 11.6                |
| Variance in statistics                    | 2.114               |
| Velocities of gas molecules               | 5.171               |
| Vinyl polymers:                           |                     |
| description of                            | 10.20               |
| properties of                             | 10.54               |
| Virial equation of state for gases        | 5.170               |
| Viscosity:                                |                     |
| of aqueous glycol solutions               | 5.138               |
| of chromatographic solvents               | 11.16               |
| conversions                               | 2.82                |
| discussion of                             | 5.137               |
| of inorganic compounds                    | 5.130               |
| of organic compounds                      | 5.90                |
| of sucrose solutions                      | 5.138               |
| of water at various temperatures          | 5.134               |
| Voltammetric half-wave potentials:        |                     |
| of inorganic materials                    | 8.141               |
| of organic materials                      | 8.146               |
| Volume:                                   |                     |
| critical                                  | 6.143               |
| factors for simplified computation of     | 11.104              |
| of geometric objects                      | 2.109               |
| Volume resistivity (dc) of polymers       | 10.22               |
| Volumetric analysis                       | 11.74               |
| Volumetric factors                        | 11.76               |
| Volumetric flasks, tolerances for         | 11.102              |
| Volumetric primary standards:             |                     |
| acid-base titrations                      | 11.74               |
| complexometric titrations                 | 11.91               |
| precipitation titrations                  | 11.94               |
| for redox titrations                      | 11.82               |
| Vulcanization and curing                  | 10.7                |
| Water:                                    |                     |
| absorption by polymers                    | 10.22               |
| binary azeotropes with                    | 5.58                |
| boiling points of                         | 5.57                |
| compressibility of                        | 5.150               |

| <b><u>Index Terms</u></b>                                         | <b><u>Links</u></b> |
|-------------------------------------------------------------------|---------------------|
| Water ( <i>Cont.</i> )                                            |                     |
| conductivity of pure, at various temperatures                     | 8.168               |
| density at various temperatures                                   | 5.87                |
| dielectric constant, refractive index, surface tension, viscosity | 5.134               |
| ion product constant of, at various temperatures                  | 8.6                 |
| ternary azeotropes with                                           | 5.79                |
| vapor pressure of                                                 | 5.28                |
| Water vapor:                                                      |                     |
| gas permeability of polymers and rubbers                          | 10.66               |
| mass of in saturated air                                          | 5.156               |
| Wavelength:                                                       |                     |
| defined                                                           | 7.38                |
| maxima of acid-base indicators                                    | 8.116               |
| to wavenumber conversion, table                                   | 2.101               |
| and X-ray tube voltage relationship                               | 7.39                |
| Wavenumber to wavelength conversion, table                        | 2.101               |
| Waxes, properties of                                              | 10.72               |
| Weighings in air to weighings in vacuo, conversion of             | 2.83                |
| Weights, analytical, tolerances for                               | 11.71               |
| Wet and dry bulb thermometer readings and relative humidity       | 11.8                |
| Wien displacement constant                                        | 2.5                 |
| Wien displacement law                                             | 7.38                |
| Wijs solution for iodine number                                   | 11.121              |
| Wine and must hydrometer                                          | 2.68                |
| Woodward-Fieser rules                                             | 7.19                |
| Work functions of elements                                        | 4.80                |
| Writing formulas of inorganic compounds                           | 3.1                 |
| Xenon:                                                            |                     |
| bond dissociation energies                                        | 4.52                |
| solubility in water at various temperatures                       | 5.8                 |
| X-ray absorption edges, wavelengths of                            | 7.5                 |
| X-ray absorption energies, critical                               | 7.8                 |
| X-ray emission energies                                           | 7.10                |
| X-ray emission spectra                                            | 7.3                 |
| X-ray filters                                                     | 7.14                |
| X-ray lines, mass absorption coefficients for                     | 7.16                |
| X-ray methods                                                     | 7.2                 |
| X-ray spectroscopy, analyzing crystals for                        | 7.15                |
| X-ray tube voltage and wavelength relationship                    | 7.39                |
| Xylenol orange, formation constants with                          | 8.104               |
| Ytterbium, bond dissociation energies                             | 4.52                |
| Yttrium, bond dissociation energies                               | 4.52                |
| Zeeman splitting constant                                         | 2.4                 |
| Zinc:                                                             |                     |
| bond dissociation energies                                        | 4.52                |
| gravimetric factors                                               | 11.66               |

**Index Terms****Links**

Zincon, formation constant with  
Zirconium:  
    bond dissociation energies  
    gravimetric factors  
z statistics

8.104  
  
4.53  
11.67  
2.120